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**Solution of Maxwell's Equations
Using the Time Domain Method of Moments
Final Technical Report
Supplement - publications and reports**

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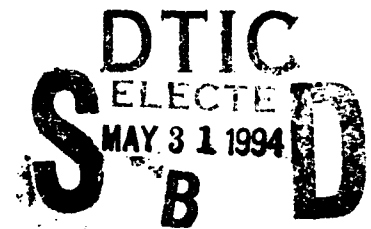
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**EIGENFUNCTION EXPANSION TECHNIQUES
IN TIME DOMAIN
(internal report) – April 1994.**

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ABSTRACT

A new approach to the analysis of Maxwell equations in the time domain is presented. The salient feature of the method discussed is that they are based on the expansion of unknown functions into infinite series of entire domain or entire subdomain basis functions and the expansion coefficients are found by means of the method of moments procedure. Four new explicit algorithms are introduced and discussed. The stability condition is derived in the general way based on the functional analysis techniques. An fast and efficient absorbing boundary condition is proposed. The results of the numerical tests are presented showing that new algorithms can achieve greater speed than a traditional FDTD technique.

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1 THEORY

1.1 Background

So far we have been considering the frequency domain formulations of the internal electrodynamic eigenvalue problems. The Fourier transform introduces the equivalence between time and frequency. Therefore each problem involving one of these quantities has two alternative representations. The time domain formulation is often used in computational physics where its potential for solving parabolic and hyperbolic differential equations arising in diffusion, convection, conductivity or oscillatory problems was recognized many years ago [18] but in electromagnetics the frequency domain formulations have traditionally been preferred for the analysis of Maxwell equations. In recent years time domain techniques have increasingly been gaining audience also in the computational electromagnetics community. Time domain algorithms solve initial value problems, but this does not mean that eigenvalue problems are not covered by time domain formulations because eigenvalues can be extracted from the time response through signal processing techniques. One advantage of the time domain methods is that they allow the investigation of transient phenomena. Additionally, they allow in principle a simple and wideband treatment of nonlinear and nonstationary processes. The disadvantage of the time domain approach is associated mainly with the difficulties in dealing with frequency dispersive materials.

The time domain analysis can be carried out based either on differential or integral formulations. The integral formulations, which are particularly attractive for scattering and radiation problems, suffer from the fact that their numerical solution is usually difficult and often accumulates discretization errors which in turn leads to instabilities [1]. For certain geometries of the scatterers it was possible to overcome these problems and develop efficient algorithms [2]. However, the difficulties associated with the integral formulations are absent in algorithms for solving differential operators and consequently most research in the area of time domain modelling of electromagnetic fields was concerned with three versatile and simple methods based on differential representations. These three algorithms are known as the Transmission Line Matrix (TLM), Spatial Network (SN) and Finite Difference - Time Domain (FDTD) methods. All three techniques are well described in the open literature [3]–[9], books [32] and monographies [20]. In the TLM and SN methods the structure under investigation is treated as a spatial network of transmission lines and the wave propagation is described by incident and reflected voltage impulses on the mesh lines. In the standard FDTD method the Maxwell's equations are discretized both in space and time, the derivatives are computed by means of central difference scheme and the fields are evaluated at discrete nodes. Although FDTD and TLM (SN) methods use different concepts and are concerned with different physical quantities, recent study by Celuch and Gwarek [10] shows that each of them can be obtained from the other by a sequence of suitable transformations. Hence, time domain methods currently used in practice are formally equivalent. Their salient feature is that three dimensional space is discretized and a mesh is formed. Samples of relevant quantities at mesh points are used to represent a physical continuum. The sampling of the solution in space is one of possible forms of a discrete representation of a physical continuum, characteristic for the approach which we called domain division. Alternative technique is to use series of entire domain and entire subdomain expansion functions to approximate the field. Let us look at time domain algorithms from the point of view of the alternative representation of fields in order to find formulations which may broaden the range of options available for the time domain analysis of complex problems of electromagnetics.

1.2 Series expansion with respect to all space coordinates

Let us consider the structure shown in fig. 1. It is assumed that the inhomogeneity is described by the relative permittivity ϵ_r and permeability μ_r , both being in general functions of all three space coordinates but frequency independent. Under these assumptions the Maxwell's equations are given by:

$$\begin{aligned}\frac{\partial}{\partial t} \vec{E} &= \frac{1}{\epsilon_0 \epsilon_r(x, y, z)} \nabla \times \vec{H} \\ \frac{\partial}{\partial t} \vec{H} &= \frac{-1}{\mu_0 \mu_r(x, y, z)} \nabla \times \vec{E}\end{aligned}\quad (1)$$

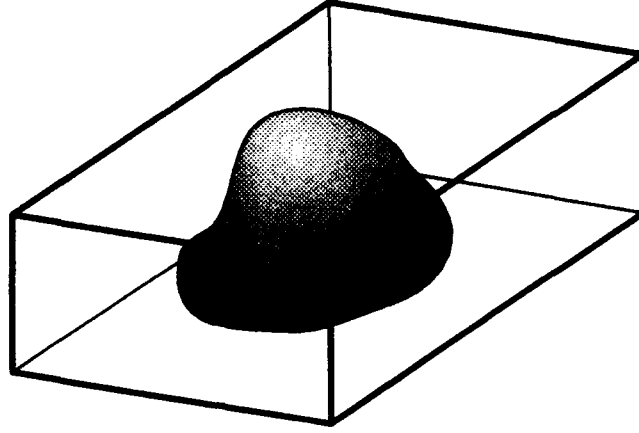


Figure 1: A cavity loaded with a dielectric inhomogeneity

These equations can be written using the following abbreviated notation

$$\begin{aligned}\frac{\partial}{\partial t} f &= L_1 g \\ \frac{\partial}{\partial t} g &= L_2 f\end{aligned}\quad (2)$$

where $L_1 = \frac{1}{\epsilon_0 \epsilon_r(x,y,z)} \nabla \times (\cdot)$, $L_2 = \frac{-1}{\mu_0 \mu_r(x,y,z)} \nabla \times (\cdot)$ and f and g are vector functions representing the electric and magnetic field, respectively. The above notation will be used henceforth.

Replacing the time derivatives with their finite difference equivalents we get the following marching on time equations

$$\begin{aligned}f^n &= f^{n-1} + \Delta t L_1 g^{n-1/2} \\ g^{n+1/2} &= g^{n-1/2} + \Delta t L_2 f^n\end{aligned}\quad (3)$$

The unknown functions f, g are now expanded into series of functions.

$$f^n = \sum a_i^n f_i(x, y, z) \quad g^n = \sum b_i^n g_i(x, y, z) \quad (4)$$

The set of expansion functions is assumed to be complete and the functions are linearly independent. The functions are defined on the entire domain or have local supports but they are in general the time independent functions of all three spatial variables. Substituting (4) into (3) we get

$$\begin{aligned}\sum a_i^n f_i &= \sum a_i^{n-1} f_i + \Delta t L_1 \sum b_i^{n-1/2} g_i \\ \sum b_i^{n+1/2} g_i &= \sum b_i^{n-1/2} g_i + \Delta t L_2 \sum a_i^n f_i\end{aligned}\quad (5)$$

Taking the inner product of (3) with the expansion functions f_i and g_i results in

$$\begin{aligned}\langle f^n, f_i \rangle &= \langle f^{n-1}, f_i \rangle + \Delta t \langle L_1 g^{n-1/2}, f_i \rangle \\ \langle g^{n+1/2}, g_i \rangle &= \langle g^{n-1/2}, g_i \rangle + \Delta t \langle L_2 f^n, g_i \rangle\end{aligned}\quad (6)$$

Using (5) the above equations can be cast into the following matrix form

$$\begin{aligned}\underline{a}^n &= \underline{a}^{n-1} + \Delta t \underline{C}^{-1} \underline{A} \underline{b}^{n-1/2} \\ \underline{b}^{n+1/2} &= \underline{b}^{n-1/2} + \Delta t \underline{D}^{-1} \underline{B} \underline{a}^n\end{aligned}\quad (7)$$

where \underline{a} and \underline{b} are the vectors containing expansion coefficients and \underline{A} , \underline{B} , \underline{C} , \underline{D} are matrices with elements given by the following inner products

$$\begin{aligned} A_{ij} &= \langle L_1 g_j, f_i \rangle & B_{ij} &= \langle L_2 f_j, g_i \rangle \\ C_{ij} &= \langle f_j, f_i \rangle & D_{ij} &= \langle g_j, g_i \rangle \end{aligned} \quad (8)$$

All matrices defined above are in general dense. If the expansion functions are orthonormal then \underline{C} and \underline{D} are identity matrices and (7) becomes

$$\begin{aligned} \underline{a}^n &= \underline{a}^{n-1} + \Delta t \underline{A} \underline{b}^{n-1/2} \\ \underline{b}^{n+1/2} &= \underline{b}^{n-1/2} + \Delta t \underline{B} \underline{a}^n \end{aligned} \quad (9)$$

1.3 Series expansion with respect to selected space coordinates

So far we have presented the algorithms in which the time is discretized and the function expansion is done in three dimensions. We shall call them total expansion algorithms. For the case when eigenfunctions of a Laplace operator are used as a basis we will use the acronym TEE (Total Eigenfunction Expansion). Another version of the expansion algorithm is obtained if the discretization is in time and one (or two) selected coordinate and the expansion is done with respect to two (or one) remaining coordinates. We shall present here a case when one space coordinate is discretized. The extension of this algorithm to the case when two space coordinates are discretized and the expansion is carried out only for the third one is straightforward. The space is sliced into subdomains (fig. 2) and the fields are expanded on each

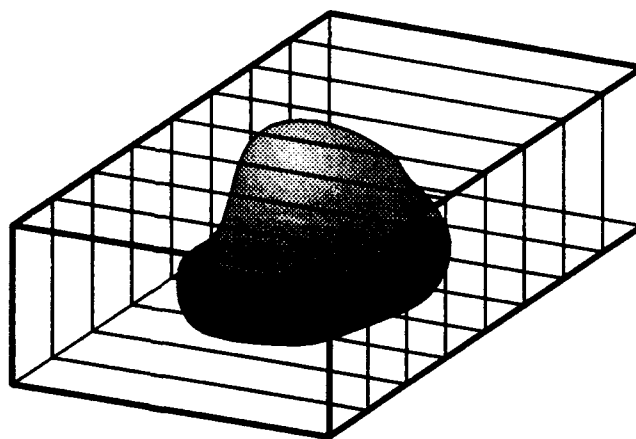


Figure 2: A structure discretized along one coordinate

subdomain (slice) into series of expansion functions. This type of expansion we shall call partial and for the eigenfunction expansion use the name the Partial Eigenfunction Expansion (PEE). To obtain the time marching equations for such case we have to introduce the finite difference scheme for the calculation of the space derivatives with respect to the discretized variable. Suppose the structure was divided into K slices in the z direction and the slices are uniformly spaced by the distance Δd . To enable the application of the central finite difference scheme for the calculation of the derivatives in the z direction we use the technique used in the FDTD method. In this technique [4] different field components are defined on two meshes, each off by half the space step from the other. This arrangement is known as the Yee's mesh. In the present context Yee's mesh is given in one spatial dimension, which means that relevant field components are defined on the slices that are off by half the space step. More precisely the E_x^k, E_y^k, H_z^k are given at $z = k\Delta d$ and H_x^k, H_y^k, E_z^k are defined for $z = (k + 1/2)\Delta d$. Bearing this convention in mind

we expand fields at a suitably situated slice according to

$$f_k^n = \sum a_{i_k}^n f_{i_k}(x, y) \quad g_k^n = \sum b_{i_k}^n g_{i_k}(x, y) \quad k = 1 \dots K \quad (10)$$

The derivatives in the z direction are approximated by

$$\frac{\partial}{\partial z} \psi_{k+1/2} \approx \frac{\psi_{k+1} - \psi_k}{\Delta d} \quad (11)$$

Calculation of the z -derivatives involves operations on the functions defined on the adjacent slices. Therefore, instead of equations (2) we get

$$\begin{aligned} \frac{\partial}{\partial t} f_k &= L_{1t}^k g_k + L_{1z}^k (g_{k+1} - g_k) \\ \frac{\partial}{\partial t} g_k &= L_{2t}^k f_k + L_{2z}^k (f_k - f_{k-1}) \end{aligned} \quad (12)$$

Where we have split operators L_1 and L_2 into transverse and z - part according to

$$\begin{aligned} L_{1t}^k &= \frac{1}{\epsilon_0 \epsilon_r^k(x, y)} \nabla_t \times (\cdot) & L_{1z}^k &= \frac{1}{\epsilon_0 \epsilon_r^k(x, y) \Delta d} \hat{z} \times (\cdot) \\ L_{2t}^k &= \frac{-1}{\mu_0 \mu_r^k(x, y)} \nabla_t \times (\cdot) & L_{2z}^k &= \frac{-1}{\mu_0 \mu_r^k(x, y) \Delta d} \hat{z} \times (\cdot) \end{aligned} \quad (13)$$

In the above equations by \hat{z} we have denoted a unit vector in the z direction.

Replacing time derivatives by the finite difference scheme, expanding functions in (12) and taking the inner products for each slice we arrive to the set of equations similar to (7) with the block diagonal coefficient matrices given by

$$\begin{aligned} \underline{A} &= \text{qdiag} [\underline{A}'^k, \underline{A}''^k] & \underline{B} &= \text{qdiag} [\underline{B}'^k, \underline{B}''^k] \\ \underline{C} &= \text{qdiag} [\underline{C}^k] & \underline{D} &= \text{qdiag} [\underline{D}^k] \end{aligned} \quad (14)$$

The elements of the submatrices are given

$$\begin{aligned} A_{ij}'^k &= \langle (L_{1t}^k - L_{1z}^k) g_{j_k}, f_{i_k} \rangle & A_{ij}''^k &= \langle L_{1z}^k g_{j_{k+1}}, f_{i_k} \rangle \\ B_{ij}'^k &= \langle (L_{2t}^k + L_{2z}^k) f_{j_k}, g_{i_k} \rangle & B_{ij}''^k &= - \langle L_{2z}^k f_{j_{k-1}}, g_{i_k} \rangle \\ C_{ij}^k &= \langle f_{j_k}, f_{i_k} \rangle \\ D_{ij}^k &= \langle g_{j_k}, g_{i_k} \rangle \end{aligned} \quad (15)$$

For orthonormal basis functions matrices \underline{C} and \underline{D} become identity matrices and we get again (9). Thus both total and partial time-domain expansion algorithms are formally described by the same set of equations (7) or (9). However, one important difference between the total and partial expansion algorithms is that in the former the matrices (8) are in general dense while in the latter the matrices (15) are always quasi diagonal.

1.4 Numerical cost of the time domain expansion algorithms

One drawback of the expansion algorithms presented in the previous section is that they may lead to higher numerical cost than FDTD and TLM. The inner products appearing in (8) and (15) are independent of time and can be stored in look up tables. If the cost of the calculation of inner products is neglected then the cost of one time step of the algorithms is determined by the cost of matrix multiplication. Depending on the basis functions used (local support versus entire domain) the overall cost may vary considerably. Generally speaking, assuming that expansion is done using L functions, the cost of one time step is of order $O(L^2)$. If the matrices are sparse the cost is lower. In the FDTD and TLM method with N nodes, the numerical cost is of order $O(N)$. Consequently, expansion techniques are comparable in terms of numerical cost and memory to classical time domain algorithms when $L^2 \sim N$. This condition will

easily be fulfilled in slightly and moderately perturbed homogeneous structures when eigenfunctions of an underlying Laplace operator are used as the expansion basis. The expansion functions have then the space distribution of the relevant field components of modes in the corresponding homogeneous problem. Similar conclusion can be derived regarding memory requirements. An important special case is when the submatrices are diagonal. This takes place for homogeneous regions (or slices) when the eigenfunction expansion is used. The numerical cost is then of order $O(L)$ which means that the expansion algorithm is faster than FDTD and TLM provided $L < N$. While in the total expansion technique this case has little practical importance, it can be very effectively used in the partial expansion algorithm as shown in Sections 1.5, and 2.1.

At this point it is important to note that a very efficient implementation of the expansion algorithms may be obtained if the expansion functions are sines and cosines. Let us consider the total expansion algorithm described by (9). Equations(6) imply that at each step one evaluates the inner products $\langle L_1 g^{n-1/2}, f_i \rangle$ and $\langle L_2 f^n, g_i \rangle$ and these inner products are used to update expansion coefficients. For sine and cosine functions the inner product for all testing functions can be computed in a very efficient way using the technique described in [13]. In this technique all the inner products are computed in one step in a sequence of inverse and forward FFTs. The procedure consists of three steps which for the total eigenfunction expansion are

- using inverse 3D FFT and $\underline{b}^{n-1/2}$ and \underline{a}^n calculate $g^{n-1/2}$, f^n and their spatial derivatives
- Compute functions $L_1 g^{n-1/2}$ and $L_2 f^n$
- using forward 3D FFT compute all inner products $\langle L_1 g^{n-1/2}, f_i \rangle$ and $\langle L_2 f^n, g_i \rangle$

Similar procedure can be used for the partial eigenfunction expansion algorithm with the 3D FFTs replaced with the 2D transforms. The numerical cost of computations of inner products using FFT was discussed in detail in [13] and depends on the number of expansion functions, number of sampling points and the inhomogeneity size but generally it is relatively low ($O(n \log_2 n)$), with n proportional to the number of unknowns) and additional advantage is that there is no need to create a look up matrices \underline{A} and \underline{B} . Again, if the number of expansion functions is low the time domain algorithms based on the eigenfunction expansions can be implemented using little computer storage and with the speed comparable to that of the corresponding FDTD or TLM methods. It should be noted however, that for large inhomogeneities, when many basis functions are needed, the performance of the function expansion codes will be worse than traditional techniques.

1.5 Hybrid expansion algorithms

The discussion of the numerical cost involved in the time domain method of moments algorithms implies that the application of the entire domain expansion functions makes sense only for moderate perturbation. This deficiency can be overcome by modifying the algorithms so that different techniques can be used in the different parts of computational space. It seems that the partial expansion algorithm offers interesting possibilities, especially with regard to problems of scattering inside waveguides (total expansion algorithms can only be applied to cavities).

1.5.1 A hybrid PEE-FDTD algorithm

Consider combining the partial expansion method with a classical FDTD algorithm. The strategy to obtain an optimal algorithm would be following. Use FDTD in the regions in which a fine resolution of field is necessary (eg. near edges, media interfaces) or large perturbation exists and apply partial expansion in the homogeneous or slightly inhomogeneous regions. Let us consider the benefits which may be obtained from this approach. In principle any complete set of functions can be used in the partial expansion algorithms, but we shall concentrate on the case when the eigenfunction expansion (PEE) is used in homogeneous regions. Let us recall that in the PEE expansion functions are chosen in such a way that they constitute a set of eigenfunctions of the Laplace operator defined on 2D region forming a slice. In that case each expansion function satisfies the boundary condition and field equations globally over entire slice and additionally, because the eigenfunctions of Laplace operator are orthogonal, matrices \underline{A}'^k , \underline{A}''^k and \underline{B}'^k , \underline{B}''^k are diagonal for homogeneous slices and the computations become extremely fast

(no more than 9 multiplications and 18 additions per iteration per 6 expansion coefficients for sine and cosine basis functions). If the PEE were also used in inhomogeneous slices, the speed of the algorithm would decrease. However if a classical FDTD algorithm is used in inhomogeneity region the numerical cost will be, locally, the same as the cost of an orthodox FDTD. Outside the inhomogeneity the PEE algorithm ensures not only fast computation but also minimizes the memory usage. This is because the eigenfunctions of the Laplace operator are selected as the basis for expansion and therefore very few series terms at each slice would be necessary to represent field in homogeneous region.

The concept of the hybrid algorithm PEE-FDTD is shown in fig.3. The two algorithms are interfaced

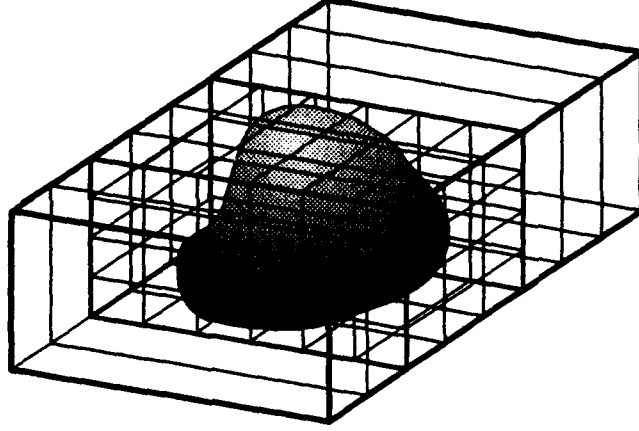


Figure 3: The mesh arrangement in a hybrid algorithm

at a common slice (say $z = z_k$) where the finite difference and partial eigenfunction expansion meshes meet. The transition from the FDTD to PEE is done in the following way. Given a field distribution at the $z = z_k$, provided by the FDTD part of the algorithm, the expansion coefficients at this slice are found by taking the inner product with each basis function of the PEE. The inner products can be calculated using numerical integration for a general case, or, for Fourier series field representation, the FFT procedures can be used. To switch from PEE to FDTD the series (10) (through direct summation or FFT) are calculated at the interface plane at the points required by FDTD.

1.5.2 A hybrid scalar PEE-vector FDTD algorithm

The time domain algorithms presented so far were formulated on Yee's mesh which is convenient for the modeling of vector fields described by Maxwell's equation. The Maxwell's equations involve 3 electric and 3 magnetic field components which means that at least 6 variables per cell are needed to characterize the fields at each iteration. Recently, Aoyagi and al [21] noted that if the electric field is divergence free, the Maxwell's equation can be converted to a set of three scalar second order equations. As shown in [21] this fact can be used in a classical FDTD algorithm to reduce both the memory and numerical cost of the algorithms. If a scalar wave approach is applied to the PEE algorithm even greater savings can be achieved. For homogeneous sections of the structure the field is a mixture of the TE and TM modes and as we noted in the previous sections each mode can be treated separately. The propagation of TE and TM modes is governed by a scalar wave equation which in the time domain is given by

$$\nabla_t^2 \phi + \left(\frac{\partial^2}{\partial z^2} - v^{-2} \frac{\partial^2}{\partial t^2} \right) \phi = 0 \quad (16)$$

where ϕ is a scalar potential whose transverse part satisfies the Neumann or Dirichlet boundary conditions and v is the velocity of light in the medium. It can immediately be recognized that the transverse part of a scalar potential can be used as the expansion term in the PEE algorithm. Consequently for each

eigenfunction ϕ_i , at each homogeneous slice we have

$$\delta_i^2 \phi_i + \left(\frac{\partial^2}{\partial z^2} - v^{-2} \frac{\partial^2}{\partial t^2} \right) \phi_i = 0 \quad (17)$$

where δ_i^2 is a transverse wavenumber. The differentiation with respect to z and t is approximated by the finite difference expressions yielding

$$v^2 \delta_i^2 \phi_{i_k}^n - (\Delta t)^{-2} (\phi_{i_k}^{n+1} - 2\phi_{i_k}^n + \phi_{i_k}^{n-1}) + v^2 (\Delta d)^{-2} (\phi_{i_{k+1}}^n - 2\phi_{i_k}^n + \phi_{i_{k-1}}^n) = 0 \quad (18)$$

This leads to an explicit algorithm

$$\phi_{i_k}^{n+1} = [2 + v^2 \delta_i^2 \Delta^2 t - 2v^2 (\Delta d)^{-2} \Delta^2 t] \phi_{i_k}^n + v^2 (\Delta d)^{-2} \Delta^2 t (\phi_{i_{k+1}}^n + \phi_{i_{k-1}}^n) - \phi_{i_k}^{n-1} \quad (19)$$

Or in a more compact form

$$\phi_{i_k}^{n+1} = A \phi_{i_k}^n + B (\phi_{i_{k+1}}^n + \phi_{i_{k-1}}^n) - \phi_{i_k}^{n-1} \quad (20)$$

where A and B are coefficients. It is important to note that each time step requires only two variables per slice and is realized with only 5 floating point operations per slice. (NB. Modern computers achieve comparable speed in addition and multiplication [34]). A vector PEE algorithm requires 6 variables per slice and 27 floating point operations under the same conditions (homogeneous slice). These parameters have to be compared with other 3D implementations of time domain techniques which require, under the most favorable conditions, at least six variables per cell and from 21 [21] to 30 [34] floating point operations per cell per iteration. Even if we disregard the fact that the PEE uses only a low number of functions in the homogeneous regions, the number of floating point operations required for one iteration makes the scalar PEE three times more efficient in terms of memory and from 4 to 6 times faster than any other published scheme. Obviously, in this comparison one has to bear in mind that the scalar PEE is applicable only to homogeneous slices. For the remaining parts of the structure one has to use the vector finite-difference time domain algorithm. To interface the two algorithms a common slice has to be chosen and either the amplitudes of scalar potentials have to be calculated from the field vectors or the other way round. A common quantity (field or potential) is calculated in the same manner as for the vector hybrid algorithm discussed in the preceding section.

1.6 Stability of the time domain expansion algorithms

The time domain algorithms discussed in this study are explicit, which implies that the time step can not exceed a certain value or the computations become unstable. Presently we shall derive the stability criterion for the the total and partial expansion algorithms. Before deriving the stability criterion let us present problem (2) in the form of a hyperbolic equation. Taking the time derivative of the first equation and applying operator L_1 to the second equation we obtain.

$$\frac{\partial^2}{\partial t^2} f = L_1 L_2 f \quad (21)$$

Putting $L = -L_1 L_2$ we get

$$\frac{\partial^2}{\partial t^2} f + L f = 0 \quad (22)$$

Equation (22) is hyperbolic differential equation. Stability of the differencing schemes for parabolic and hyperbolic equations has been studied in [17] and [35] in context of classical finite difference representation of differential operators. The theorems used in that case are also applicable to the present method. To investigate the stability of time marching algorithms for the hyperbolic equations it is useful to present a problem in a canonical form

$$\Delta^2 t R \frac{\partial^2}{\partial t^2} f + A f = 0 \quad (23)$$

The time marching algorithm for the above problem is stable if the following conditions are fulfilled [17](p.386):

$$A = A^* > 0, \quad R = R^* > 0 \quad (24)$$

$$R - \frac{A}{4} \geq 0 \quad (25)$$

In other words, for the time marching algorithm to be stable it is sufficient that both operators \mathbf{A} and \mathbf{R} are self adjoint and positive and additionally the operator $\mathbf{R} - 0.25\mathbf{A}$ is nonnegative. The canonical form (23) is obtained from (22) by simply writing it as

$$\frac{\Delta^2 t}{\Delta^2 t} \mathbf{I} \frac{\partial^2}{\partial t^2} f + \mathbf{L} f = 0 \quad (26)$$

Where \mathbf{I} is the identity operator.

Comparing (26) with (23) we get $\mathbf{R} = \mathbf{I}/\Delta^2 t$ and $\mathbf{A} = \mathbf{L}$. It can readily be verified that operator \mathbf{L} is symmetric and positive. It suffices to verify the condition (25). This condition is fulfilled when

$$\|\frac{\mathbf{I}}{\Delta^2 t}\| \geq \frac{\|\mathbf{L}\|}{4} \quad (27)$$

or

$$\Delta t \leq \frac{2}{\sqrt{\|\mathbf{L}\|}} \quad (28)$$

Thus the maximal time step in explicit time domain algorithms considered here depends on the norm of the operator \mathbf{L} .

For a self-adjoint bounded operator \mathbf{L} defined in the Hilbert space \mathcal{H} the norm is defined as [36]

$$\|\mathbf{L}\| = \sup_{y \in \mathcal{H}, \|y\|=1} |\langle \mathbf{L}y, y \rangle| = |\lambda_{max}| \quad (29)$$

where λ_{max} is the largest eigenvalue of \mathbf{L} .

Let us estimate the norm of the operator \mathbf{L} . To this end we consider a simpler, one dimensional second order operator defined over an interval $0 \leq x \leq l$

$$\mathbf{F} = -b(x) \frac{\partial^2}{\partial x^2}(\cdot) \quad (30)$$

where $b(x) > 0$ is a time independent positive continuous function of x . Let \mathcal{D} denote the domain of operator \mathbf{F} and assume that it allows only square integrable functions satisfying Dirichlet conditions at both ends of the interval. Since the space of square integrable functions is infinite dimensional, the operator \mathbf{F} is unbounded and consequently its norm is infinite. It is necessary to calculate its norm in finite dimensional space. This is what happens in practice because we always look for approximate solution to the problem in a form of a linear combination of finite number of basis functions. The finite set of basis function defines the approximate finite dimensional subspace of original domain. Consider the following truncated set of basis functions

$$\sqrt{\frac{2}{l}} \sin \frac{i\pi x}{l} \quad i \leq N_M \quad (31)$$

The basis functions (31) span a finite dimensional space $\mathcal{H}_{N_M} \subset \mathcal{D}$ in which the approximate solution is sought for. Now it is easy to find the upper bound of the operator.

$$\|\mathbf{F}\| = \|b(x) \frac{\partial^2}{\partial x^2}(\cdot)\| \leq \|b_{max} \frac{\partial^2}{\partial x^2}(\cdot)\| = \|\mathbf{F}_m\| \quad (32)$$

Where b_{max} is the maximal absolute value of $b(x)$ over the interval $< 0, l >$. The eigenvalues λ_i of operator \mathbf{F}_m are given by

$$\lambda_i = \frac{i^2 \pi^2}{b_{max} l^2} \quad (33)$$

and consequently the norm of \mathbf{F}

$$\|\mathbf{F}\| \leq \frac{N_M^2 \pi^2}{b_{max} l^2} \quad (34)$$

Similar derivation can be used for \mathbf{F}_Δ , a finite difference analogue of operator \mathbf{F} yielding [17]

$$\|\mathbf{F}_\Delta\| \leq \frac{4}{(\Delta d)^2 b_{max}} \quad (35)$$

where Δd is the discretization step.

At this point we can return to operator $\|\mathbf{L}\|$. Let us consider a cube Ω with the dimensions $l \times l \times l$. We seek the approximate solution given a finite number of expansion functions in the form of normalized products of sines and cosines

$$\sin \frac{i\pi\xi}{l} \quad \text{or} \quad \cos \frac{k\pi\xi}{l} \quad i, k \leq N_M \quad (36)$$

Let \mathcal{D} denote the domain of the original problem given by equations (2). The basis functions (36) span a finite dimensional space $\mathcal{H}_{N_M} \subset \mathcal{D}$. We calculate the upper bound of the norm of operator $\|\mathbf{L}\|$. Note that $\|\mathbf{L}\| \leq \|\mathbf{L}_m\|$. Where

$$\mathbf{L}_m = (\epsilon_0 \mu_0 \epsilon_{\min} \mu_{\min})^{-1} \nabla \times \nabla \times (\cdot) \quad (37)$$

and

$$\epsilon_{\min} = \inf \epsilon_r(x, y, z), \quad \mu_{\min} = \inf \mu_r(x, y, z) \quad x, y, z \in \Omega \quad (38)$$

Using the same procedure as above we find the norm of operator \mathbf{L} in \mathcal{H}_{N_M}

$$\|\mathbf{L}\| \leq \|\mathbf{L}_m\| \leq v_{\max}^2 \frac{3N_M^2 \pi^2}{l} \quad (39)$$

where $v_{\max} = (\epsilon_0 \mu_0 \epsilon_{\min} \mu_{\min})^{-1/2}$ is the maximum velocity for a plane wave in the medium filling the structure. Using the above estimation we get the following stability condition

$$\Delta t \leq \frac{2l}{v_{\max} N_M \pi \sqrt{3}} \quad (40)$$

If Ω is a rectangular prism with the dimensions $a \times b \times l$ and the upper bound for i, l, m in the trigonometric expansion functions is K_M, L_M, N_M then the condition (40) becomes

$$\Delta t \leq \frac{2}{v_{\max} \pi \sqrt{(\frac{K_M}{a})^2 + (\frac{L_M}{b})^2 + (\frac{N_M}{l})^2}} \quad (41)$$

For partial eigenfunction expansion scheme using sine and cosine $K_M \times L_M$ basis functions over rectangular $a \times b$ slices with the discretization Δd in z direction, the stability condition derived using (35) is

$$\Delta t \leq \frac{2}{v_{\max} \sqrt{(\frac{\pi K_M}{a})^2 + (\frac{\pi L_M}{b})^2 + (\frac{2}{\Delta d})^2}} \quad (42)$$

Obviously for other separable cylindrical coordinate systems with the discretization Δd in z direction, the stability condition will be determined by the maximal value of the transverse eigenvalue (separation constant) δ_{\max}^2 as the functional analysis will give

$$\Delta t \leq \frac{2}{v_{\max} \sqrt{\delta_{\max}^2 + (\frac{2}{\Delta d})^2}} \quad (43)$$

For the discretization of all three coordinates with steps $\Delta x, \Delta y, \Delta d$ we shall get the well known Courant condition [20]

$$\Delta t \leq \frac{1}{v_{\max} \sqrt{(\frac{1}{\Delta x})^2 + (\frac{1}{\Delta y})^2 + (\frac{1}{\Delta d})^2}} \quad (44)$$

At this point it is interesting to observe that the derivation described above can be used for investigation of the stability of compact 2-D/FDTD schemes considered by Cangellaris [19]. In fact a compact 2-D/FDTD algorithm for the analysis of waveguides is a special case of one of the partial expansion algorithms presented in Section 1.3 with the space having two uniformly discretized cartesian coordinates x, y and the variation in the z direction given by one basis function of the form $\exp(-j\beta z)$. For this case we get

$$\Delta t \leq \frac{1}{v_{\max} \sqrt{(\frac{1}{\Delta x})^2 + (\frac{1}{\Delta y})^2 + (\frac{\beta}{2})^2}} \quad (45)$$

This condition is identical as the one given in [33] and [19].

Finally, let us compare the Courant condition (44), valid for the classical 3D FDTD and TLM schemes with the condition for total and partial eigenfunction expansion schemes using harmonic function expansion. For simplicity let us assume that a cubical region $a \times a \times a$ is considered with cubical lattice $\Delta x = \Delta y = \Delta z$ for FDTD and the number of expansion function in each direction is N_M for the method of moments algorithms. Let $N_\Delta = a/\Delta x$. N_Δ is then the number of discretization points along one direction. The Courant condition can be rewritten as

$$\Delta t_\Delta \leq \frac{1}{v_{max}(\frac{a}{N_\Delta})\sqrt{3}} \quad (46)$$

Comparing the above result with (40) we get the ratio of the maximum allowable time steps for the considered algorithms

$$\frac{\Delta t_M}{\Delta t_\Delta} = \frac{\pi N_M}{2 N_\Delta} \quad (47)$$

It is seen that the method of moments algorithm can operate with greater a time step than a classical FDTD scheme if

$$N_M < \frac{2}{\pi} N_\Delta \approx 0.638 \frac{a}{\Delta x} \quad (48)$$

The identical condition is obtained for the 3D partial eigenfunction expansion scheme with sine and cosine basis functions. Since the idea of the time domain expansion algorithms consists in using a fewer number of unknowns to represent the fields, the condition (48) is likely to be fulfilled in many practical situations.

1.7 Absorbing boundary conditions

One of the most important issues in treating open problems is a proper definition of the boundary conditions at the places where no physical boundary exists. This problem occurs also in the partial expansion algorithm (the total expansion can be used only in completely closed structures) when the geometries involving waveguides have to be modeled. The waveguiding structure is assumed to be uniform in the propagation direction and guided modes propagate along the structure without attenuation. Since the structure is infinite, then the application of an algorithm with the space discretization in the propagation direction would imply division into an infinite number of slices. To minimize the time of computations and reduce the computer storage, the number of slices has to be kept as small as possible. The way of achieving this is to consider only a section of a waveguide and introduce the boundary conditions at its both ends which simulate the infinitely long structure.

The problem of keeping the computational space as small as possible, is one of the most fundamental in all time domain methods using finite differencing scheme in the modeling of uniform infinite structures and is known as the problem of the Absorbing Boundary Condition (ABC) or Radiation Boundary Condition (RBC). The name Absorbing Boundary Condition comes from the physical interpretation of the conditions which model infinitely long structures. If the structure is uniform then the forward propagating wave does not give rise to any backward traveling waves. So if a section of the waveguide is considered the conditions at its extremes have to be specified in such a way that a wave impinging on them can not cause any reflection. From the point of view of an observer inside the guide the wave would get completely absorbed. Traditional FDTD schemes use usually different schemes based on the decomposition of wave equation into a operators describing one way propagation (towards or away from the boundary), approximation of the resulting operator using the Taylor series or Padé rational approximation and setting to zero the expression representing the wave travelling back to the interior of the structure [20]. This process results in the Mur's first and second order conditions [12]. Mur's conditions and their modifications are very popular in time domain analysis of open space problems when the propagation is not dispersive. In the waveguiding structures especially when the dispersion is large the Mur's ABC are not satisfactory. One approach used for highly dispersive structures is to replace waveguide by a long section of a lossy transmission line. Recent publications show [26] that with this approach the return loss better than -80dB can be obtained in the octave band at the numerical cost ranging from few hundred to few thousand memory cells and floating point operations per iteration. Alternative approach sometimes called the time domain diakoptics [22, 23] is also being considered by some authors.

1.7.1 Time domain diakoptics

The diakoptics is the technique in which a large system is first decomposed into modules, each module is analyzed separately and the solution for the complex system is achieved by finding the relation between the solutions obtained for individual modules [29]. Diakoptics, by nature of the algorithm, is particularly well suited for modern multi processor, parallel and massively parallel computers [30]. The concept of system segmentation is frequently used in network and field theory in time and frequency domain. To present this technique in the context of ABC for waveguides, we shall express the problem in the language of the theory of linear systems.

Suppose the structure is infinite in the z direction and we want to analyze the wave propagation in this direction using the partial eigenfunction expansion scheme (PEE). To this end we consider a section of the structure consisting of K slices spaced by Δd . We use Yee's mesh so that relevant fields are calculated on the slices that are off by half the space step. Calculation of the fields at last location $z = (K + 1/2)\Delta d$ requires calculation of the following expression

$$\frac{\partial}{\partial z} \psi_{K+1/2}(t_n) \approx \frac{\psi_{K+1}(t_n) - \psi_K(t_n)}{\Delta d} \quad (49)$$

This can be done only if we specify $\psi_{K+1}(t_n)$ which is equivalent to imposing an ABC at $z = (K + 1)\Delta d$. To find the value of $\psi_{K+1}(t_n)$ consider a linear system shown in fig.4.

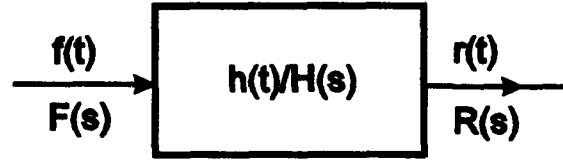


Figure 4: A linear system

The system has the transfer function $H(s)$ where s the variable of Laplace transform. The Laplace transforms of the input $F(s)$ and output $R(s)$ signals are related via

$$R(s) = F(s)H(s) \quad (50)$$

This relation can be written in the time domain as

$$r(t) = f(t) * h(t) \quad (51)$$

where $*$ is the symbol for the convolution integral and $h(t)$ is the impulse response of the system. For functions sampled at time instances $i\Delta t$, the response $r_n = r(n\Delta t)$ is evaluated by the summation

$$r_n = \Delta t \sum_{m=1}^{n-1} f_{n-m} h_m \quad (52)$$

If we assume that $r(t)$ and $f(t)$ are the fields at $z = (K + 1)\Delta d$ and $z = K\Delta d$, respectively then using (51) we may calculate the value of the field at $z = (K + 1)\Delta d$ hence imposing an ABC at the extreme slice of the guide. In the case of the PEE analysis of a waveguide the transfer function approach allows us to find the ABC by convolving the impulse response of an elementary slice of the guide of the length Δd with the field at $z = \Delta d$. Referring back to the concept of diakoptics we see that the interior of the analyzed guide and the ABC are two modules which can be analyzed separately and the response of the whole system will be given, in time domain, by the convolution. For TLM method the time domain diakoptics treatment of ABC condition was initially implemented by individually convolving signals at each point of discretization [23]. This approach is computationally inefficient so very recently it has been refined for the ABC in homogeneous guides by first converting the discrete representation of fields into modes and convolving each mode separately [24, 25]. It has to be noted that for the PEE the eigenfunction representation is an inherent feature of the algorithm so the solution of the ABC problem using time domain diakoptics seems to be a good choice.

1.7.2 Low cost algorithms for efficient implementation of absorbing boundary condition in the PEE

At this point it has to be noted that unless the impulse response is short the calculation of the convolution is very time and memory consuming. Typically around 1000 memory cells and a similar number of floating point operations at each iteration is needed to obtain low return loss. In order to reduce the computer time it is necessary to find algorithms which allow the computation of convolutions required to model ABC fast enough.

Finite impulse response approach The most straightforward approach to accelerate the computation of the convolution is to limit the duration of the impulse response. In this way an elementary section of the guide is modelled via an approximate "black box" with a finite impulse response *FIR*. Bearing in mind that the Laplace and Fourier transforms are closely related via the substitution $s = j\omega$, we may find the transfer function of a section of a waveguide the length Δd by finding its frequency response. For the time harmonic ($\exp j\omega$) fields the propagation in the z -direction is described (in the frequency domain) by the factor $\exp[-j\beta(\omega)z]$. The transfer function $H(j\omega)$ is then

$$H(s) = H(j\omega) = e^{-j\beta(\omega)\Delta d/c} = e^{-j\beta(\omega)\Delta\tau} \quad (53)$$

where $\beta(\omega)$ is the propagation constant and c is the velocity of the light. If the guide is nondispersive then $\beta(\omega) = A\omega/c$, with A being a constant, and hence

$$h(t) = \delta(t - A\Delta\tau) \quad (54)$$

where $\delta(t)$ is the Dirac function. From the above equation it can be concluded that a nondispersive guide behaves as an ideal, nondistorting all pass filter which introduces only the time delay $A\Delta\tau$. If the time step Δt in the PEE algorithm is chosen so that $l\Delta t = A\Delta\tau$, with l being an integer, then the ABC is determined by simply substituting

$$\psi_{K+1}(t_n) = \psi_K(t_{n-l}) \quad (55)$$

In other words, in a nondispersive guide the field at $z = (K+1)\Delta d$ is completely determined by the field at $z = K\Delta d$ by $l = A\Delta d/(c\Delta t)$ time instances earlier. In the dispersive guide the situation is different because in this case the impulse response may be in general infinite. If the frequency behavior of $\beta(\omega)$ is known then an approximate ABC can be obtained by taking the inverse Fourier transform of the transfer function and time limiting the impulse response, so that the convolution can be performed fast enough.

In order to illustrate this concept in more detail let us consider the electromagnetic wave propagation in a rectangular waveguide with a local inhomogeneity. The guide is excited by the bandwidth limited signal with the upper frequency limit lower than the cutoff frequency of the first higher order mode. Under these assumptions only a fundamental mode can propagate away from the inhomogeneity. If we apply the PEE method to the analysis of this guide then the expansion coefficients correspond to the mode amplitudes. The coupling between expansion functions (modes) takes place only at the slices located in the region of inhomogeneity. Outside the inhomogeneity the expansion functions are not coupled and therefore the time evolution of the expansion function can be found at a marginal numerical cost. Note that since the operating conditions allow only a single mode propagation, then if we terminate the guide sufficiently far away from the inhomogeneity, the higher order modes excited in the inhomogeneity region will die out and we will have to specify only the ABC for one propagating mode (If more than one mode would be allowed to propagate then a separate ABC would have to be specified for each propagating mode in the same way as for the fundamental mode). The dispersion characteristic of modes supported in the rectangular waveguide are known and consequently the impulse response function required for the ABC is also known

$$h(t) = \mathcal{F}^{-1}\{e^{-\gamma(\omega)\Delta d}\} \quad (56)$$

where \mathcal{F}^{-1} is a symbol denoting the inverse Fourier transform and

$$\gamma(\omega) = \sqrt{\omega_c^2 - \omega^2}/c \quad (57)$$

with c denoting the light velocity and ω_c being the cutoff angular frequency of a mode. A cylindrical waveguide is a high pass filter. From the circuit theory we may conclude that its impulse response is

$$f^n = \sum a_i^n f_i(x, y, z) \quad g^n = \sum b_i^n g_i(x, y, z) \quad (4)$$

causal. We can now consider the behavior of the impulse response. Since it is difficult to calculate the impulse response analytically we replace the section of the waveguide by an ideal nondistorting high pass filter with the stop band $(-\omega_c, \omega_c)$. The transfer function of an ideal filter is

$$H(j\omega) = (1 - G_{\omega_c}(\omega))e^{-j\omega\Delta\tau} \quad (58)$$

where $\Delta\tau = \Delta d/c$ and $G_{\omega_c}(\omega)$ is the gate function which equals unity in the stop band and vanishes outside. The impulse response can now readily be found (normalization constants neglected)

$$h(t) = \delta(t - \Delta\tau) - \frac{\omega_c \sin(\omega_c(t - \Delta\tau))}{\pi(t - \Delta\tau)} \quad (59)$$

Note that the second term's roll off is proportional to $1/t$. The distance between first zeros is $2\pi/\omega_c$, and if we truncate the impulse response at this point, the ABC will be modelled by convolving using approximately $2\pi/(\omega_c\Delta t)$ samples. The ideal filter are nonphysical and therefore their impulse responses are acausal but this analysis can be used as a guideline for determining the truncation point in real guides.

Adaptive prediction The situation is more difficult when $\beta(\omega)$ is not known. For this case let us write the transfer function of a slice of a dispersive guide as $H(s) = H_i(s)H_d(s)$ where $H_i(s)$ is the transfer function of an nondispersive guide and $H_d(s)$ represents the distortion introduced by the dispersion. In terms of the "black boxes" the section of the guide is now replaced by the cascade of an all pass nondistorting filter (a delay line) and a filter (bandwidth limited or all pass) with nonlinear phase characteristic. The $H_i(s)$ and $H_d(s)$ are defined as follows

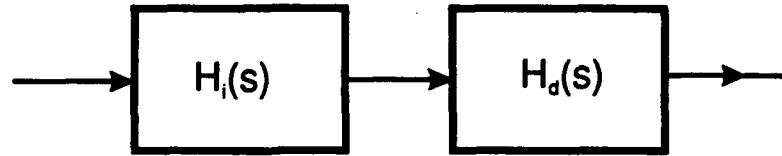


Figure 5: A system representation of a dispersive waveguide

$$H_i(s) = H_i(j\omega) = e^{-jA\omega\Delta\tau} \quad (60)$$

$$H_d(s) = H_d(j\omega) = e^{-j[c\beta(\omega) - A\omega]\Delta\tau} \quad (61)$$

In a physical waveguide the dispersion is significant at low frequency and gradually vanishes as the frequency increases. Therefore,

$$\lim_{\omega \rightarrow \infty} [c\beta(\omega) - A\omega] = 0 \quad (62)$$

The value of $\Delta\tau$ depends on the discretization step but can be arbitrarily small. Consequently, the argument in the exponent may be made small for all ω 's and the transfer function $H_d(j\omega)$ can be approximated by two term Taylor series

$$H_d(s) = H_d(j\omega) = e^{-j[c\beta(\omega) - A\omega]\Delta\tau} \approx 1 - j[c\beta(\omega) - A\omega]\Delta\tau \quad (63)$$

Let us put $P(\omega) = j[c\beta(\omega) - A\omega]\Delta\tau$. Since we are considering only causal systems ($P(\omega)$ satisfies the Paley-Wiener criterion [16]) the $P(j\omega)$ is the Fourier transform of function $p(t)$.

$$P(j\omega) = \int_0^{\infty} p(t)e^{-j\omega t} dt \quad (64)$$

If $p(t)$ is discretized in the time domain with the time step Δt the integral is replaced by the finite complex Fourier series

$$P(j\omega) \approx \sum_{i=0}^N p(i\Delta t)e^{-j\omega i\Delta t} \quad (65)$$

The transfer function of the system is then

$$H(s) \approx H_i(j\omega)(1 - P(j\omega)) = e^{-jA\omega\Delta\tau} - \sum_{i=0}^N p(i\Delta t) e^{-j\omega(i\Delta t + A\Delta\tau)} \quad (66)$$

We can now calculate the impulse response $h(t)$. The impulse response is then

$$h(t) = \delta(t - A\Delta\tau) - \sum_{i=0}^N p_i \delta(t - (i\Delta t + A\Delta\tau)) \quad (67)$$

The impulse response given above describes the cascade of a delay line and a digital filter of the order N with unknown weighting coefficients p_i . The unknown coefficients can be found using the system identification approach. One possible solution could be to select two adjacent slices located at $z = k\Delta d$ and $z = (k+1)\Delta d$, $k+1 \leq K$ which have the same cross section as slices terminating the guide. The relation between input and output signals between these two adjacent slices is the same as for the K -th and $K+1$ -st slice. We may now sample the signals at the input and output of the test section and find the set of coefficients p_i which minimizes the error between the actual response and the response predicted by (67). An advantage of using a digital filter approach is the possibility to synchronize the filter with the time step of the field modelling method. This allows one to take into account the effect of numerical dispersion. Additionally, the coefficients p_i can be computed at a low cost using recursive, self adapting algorithms [15]. It should be mentioned that system identification models have been very recently used with success to accelerate the computations of the time domain electromagnetic simulators [28] or diakoptics in which modules were modeled with classical FDTD algorithm [27].

Off line identification The evaluation of the convolution can be immensely accelerated if the response function can be represented suitably chosen discrete model. Such an approach has been already proved to be very useful in development of time domain algorithms for frequency dependent materials [20] and therefore it is useful to consider this technique for the realization of the ABC in the PEE method.

Suppose the impulse response is given by

$$h(m) = \sum_{l=1}^L a_l g_l(m) \quad (68)$$

with L and g_l being a small integer and a function defined for $0 \leq t < \infty$, respectively. Let us assume that the expansion functions are given by

$$g_l(m) = e^{-\alpha_l m} \quad (69)$$

We additionally assume that the expansion functions can be evaluated recursively so that

$$g_l(m+1) = A_l g_l(m) \quad (70)$$

with $A_l = \exp(-\alpha_l)$. The convolution is expressed then as

$$r(n) = \Delta t \sum_{m=1}^{n-1} \sum_{l=1}^L a_l g_l(m) f(n-m) \quad (71)$$

Using the recursion (70), the convolution is evaluated through a compact formula

$$r(n) = \Delta t \sum_{l=1}^L p_l(n) \quad (72)$$

where

$$p_l(n) = a_l A_l f(n-1) + A_l p_l(n-1) \quad (73)$$

It is seen that the computations are reduced to merely an update formula for p_l . For the case of frequency dependent material considered in [20], the impulse response is specified analytically so the expansion coefficients could be calculated using the Prony method. Alternatively a suitable recursion algorithm can be implemented using the off line identification process similar to the on line technique described in the preceding subsection. The advantage of the off line identification is that the ABC can be modelled prior to time domain computations and hence reduce the numerical complexity of the PEE.

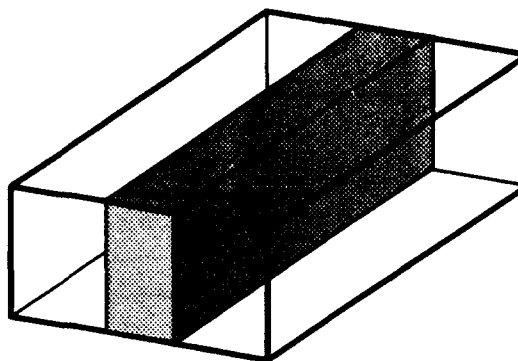


Figure 6: Geometry of a rectangular resonator loaded with a dielectric slab used in numerical test to validate TEE and PEE algorithms. The dimensions are width $a = 12\Delta d$, height $b = 6\Delta d$, length $c = 8\Delta d$, slab parameter $\epsilon_r = 3.75$, slab centered, slab with w varying.

2 VALIDATION OF THE ALGORITHMS

2.1 Time domain algorithms

All time domain algorithms presented above, except for the hybrid scalar PEE-FDTD scheme, have been implemented and tested for the case of the rectangular resonators or waveguides containing dielectric slabs. The eigenfunctions of the Laplace operator with Dirichlet or Neumann boundary conditions were used as the expansion functions and the inner products were calculated using the Fast Fourier Transform approach. The algorithms have been found stable provided the time step did not exceed the critical values given in Section 1.6. Some numerical results for the expansion algorithms with sine and cosine expansion functions are given in Table 1 where the normalized resonant frequencies $\Delta d/\lambda$ are compared for fundamental mode in a rectangular resonator obtained from a section of a waveguide shown in fig.6 using the total and partial eigenfunction expansions algorithms with the data FD-TD published in [9] and the transverse resonance method. The parameter Δd is the discretization step used in the FDTD and PEE algorithms. The agreement is very good for all cases included in the table. Subsequently a

Table 1: Comparison of the results for the normalized resonant frequencies $\Delta d/\lambda$ obtained using expansion algorithms with the published data [9] for the rectangular resonator with a dielectric slab (fig.6)

	TRM	Partial Expansion	Total Expansion	FD-TD[9]
$w = 0$	0.07511 (exact)	0.07502	0.07511	0.0750
$w = 2\Delta d$	0.0522	0.05253	0.05153	0.0517
$w = 4\Delta d$	0.0445	0.04456	0.04433	0.0442

hybrid vector PEE-FDTD algorithm presented in Section 1.5.1 was tested. For this algorithm the cutoff frequency of the EH_{11} of a rectangular guide loaded with a dielectric slab shown in fig.7 was computed and compared with the results obtained with a classical FDTD technique. The dimensions of the guide were taken to be 20 by 6 mm. The slab is placed on the wider wall in the symmetry plane of the structure and has the width 4mm and relative permittivity of 2.5. Three cases were considered corresponding to the slab height of 0, 4 and 6 mm. Although the structure is symmetric, the symmetry was not exploited during the computation. In all tests the identical excitation, space discretization ($\Delta d = .5mm$, time step, $\Delta t = .9\Delta d/(c_0\sqrt{2})$), and number of samples $N = 8000$ were assumed. The results are given in Tables 2 and 3 together with the CPU time for a DELL 466/L personal computer. For the FDTD algorithm alone the CPU time for the assumed discretization mesh was 53s and was identical for all three cases.

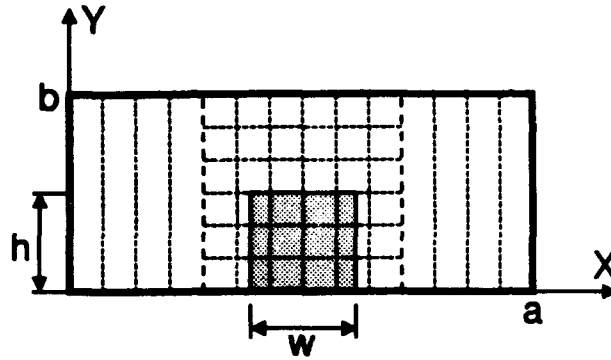


Figure 7: Geometry of a rectangular guide loaded with a dielectric slab used to validate the vector hybrid time domain method of moments showing PEE and FDTD meshes

Table 2: Comparison of the results and CPU times for the cutoff frequencies of EH_{11} mode in the 20 by 6 mm rectangular guide loaded with a dielectric slab ($\epsilon_r = 2.5$, $w = 4$ mm, h - varying) using only FDTD and PEE algorithms for number of expansion functions N and the localization of the interface planes as parameters

Slab height	FDTD	CPU	PEE	CPU
$h = 0$ mm	26.0475 GHz	53s	26.0625 GHz	2s
$h = 6$ mm	19.9075 GHz	53s	19.0375 GHz	2s
$h = 4$ mm	20.1875 GHz	53s		

For the slab height of 0 mm and 6 mm and the discretization along the wider side of the waveguide, it is possible to use PEE algorithm with homogeneous slices only. Since only one expansion function is needed for the mode considered, the CPU time is 2s or 26.5 times faster than the FDTD. For the slab height of 4 mm slices in the slab region are inhomogeneous and therefore the hybrid vector PEE-FDTD algorithm was used. The slab region was treated with the FDTD and the lateral homogeneous regions were calculated with PEE. The CPU time depends on the localization of the interface plane and the number of expansion functions used in the PEE part of the algorithm. When the interface is at $x_1 = 7.5$ and $x_2 = 12.5$ mm, i.e. when the FDTD mesh is terminated only one slice away from the inhomogeneous region, the CPU time of the hybrid algorithm varies from 18s (for 1 expansion function) to 27s (for 5 expansion functions), with most of the time (14s) consumed by the FDTD computations. The error introduced by low number of expansion functions is the largest if only one term is used but for this structure is lower than 0.1% compared the result obtained from pure FDTD calculations. The error decreases as the interface plane is moved away from the inhomogeneity. This is due to the fact that higher order terms in the field expansion correspond to higher order waves traveling in the lateral direction. These modes are attenuated so their contribution to the field of the EH_{11} mode becomes less significant. If the interface planes are located at $x_1 = 5$ and $x_2 = 15$ mm, only one term in the PEE part is sufficient to obtain exactly the same results as with purely FDTD technique. The CPU time for this case is 31s of which 28s is spent in the FDTD part. The increase in the number of expansion terms does not change the results.

No tests so far have been carried out for the hybrid scalar PEE-FDTD discussed in Section 1.5.2 but since scalar version of PEE it is about 5 times faster than a vector algorithm even larger speed up factors may be expected for the structure considered above.

Table 3: Comparison of the results and CPU times for the cutoff frequencies of EH_{11} mode in the 20 by 6 mm rectangular guide loaded with a dielectric slab $\epsilon_r = 2.5$, $w = 4\text{mm}$, $h = 4\text{mm}$ using a hybrid algorithm with the number of expansion functions N and localization of the interface planes as parameters

N	PEE-FDTD [GHz]	Error rel. to FDTD	CPU FDTD part	CPU PEE part	CPU combined	Speed up rel. to FDTD (53s)
Interface of algorithms at $x = 7.5, x = 12.5$ mm						
1	20.2075	+ 0.1%	14s	4s	18s	2.9
3	20.1975	+0.05%	14s	9s	23s	2.3
5	20.1975	+0.05%	14s	13s	27s	1.96
Interface of algorithms at $x = 6.5, x = 13.5$ mm						
1	20.195	+0.025 %	19s	4s	23s	2.3
3	20.1925	+0.01%	19s	8s	27s	1.96
Interface of algorithms at $x = 5, x = 15$ mm						
1	20.1875	0%	28s	3s	31s	1.7
3	20.1875	0%	28s	6s	34s	1.55

2.2 Absorbing boundary condition

The absorbing boundary condition was implemented for the case of the TE_{10} mode in a rectangular waveguide. The off line identification procedure consisting in expanding the dispersive part of the impulse response into series of the Leguerre polynomials was used to model the dispersive part of the waveguide. The expansion can be written in the following form

$$h_d(t) = \sum_{i=1}^p c_i L_i(t) \quad (74)$$

where $L_i(t)$ denotes the Leguerre polynomial of the order i . The Leguerre polynomials have the advantage of yielding an always stable model. Prior to simulation a wide band signal shown in fig.8 was propagated using the PEE algorithm for 600 time steps and its samples taken at two adjacent slices were recorded. Based on this data the expansion coefficients in (74) were found and used during the actual simulations. Fig.9 shows the return loss of the ABC in a 10.16 by 22.86mm rectangular waveguide. The solid, dashed and dashed dotted lines correspond to $p = 2$, $p = 5$ and $p = 10$ in expansion (74), respectively. It is seen that even for the lowest approximation order the results are excellent as the return loss is lower than -80 dB over a very wide frequency band. The worst performance is seen near the cutoff frequency. Fig.10 shows the close up of the cutoff region it is seen that increasing the approximation order the the quality of the ABC improves quickly. Since the practical structures do not operate at cutoff frequency -20 dB return loss at this point will have no influence on actual modeling. It should be noted that the numerical cost of implementing the proposed ABC is extremely low. The overhead is marginal as the calculation of response requires only a few times the number of expansion terms of extra floating point operations and the storing the a few expansion coefficients. It has to be noted that this cost is a few orders of magnitude lower than in the most recently published results [23, 25, 24, 26] of the other authors, where form few hundreds to few thousand of extra floating point operations at each time step and a similar number of additional memory locations was used to achieve a similar performance of ABC.

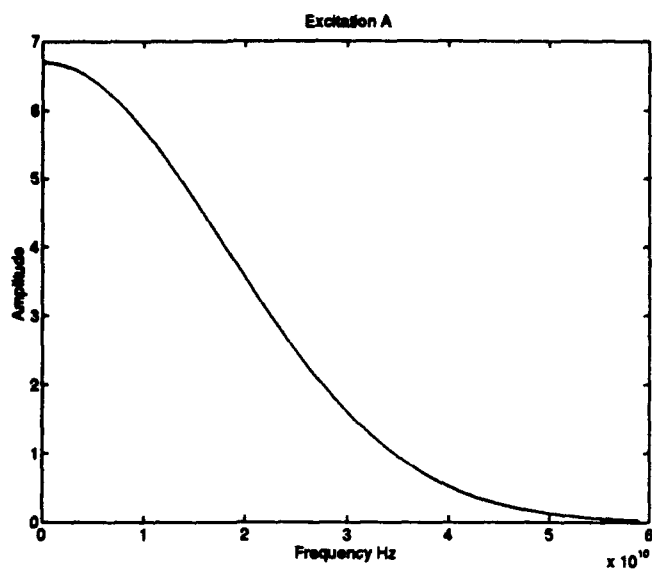


Figure 8: The excitation used for off line identification of the ABC

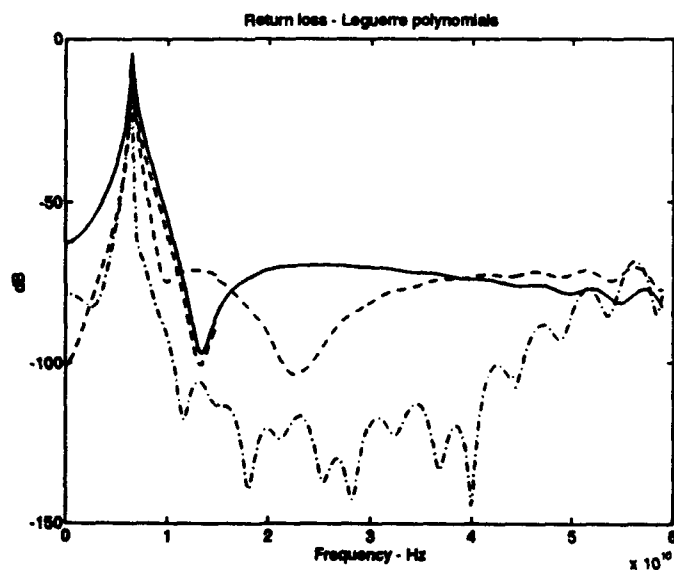


Figure 9: The return loss of the ABC for a TE_{10} mode in a 10.16 by 22.86mm rectangular waveguide. The solid, dashed and dashed dotted lines correspond to two, five and ten Laguerre polynomials used in expansion (74), respectively

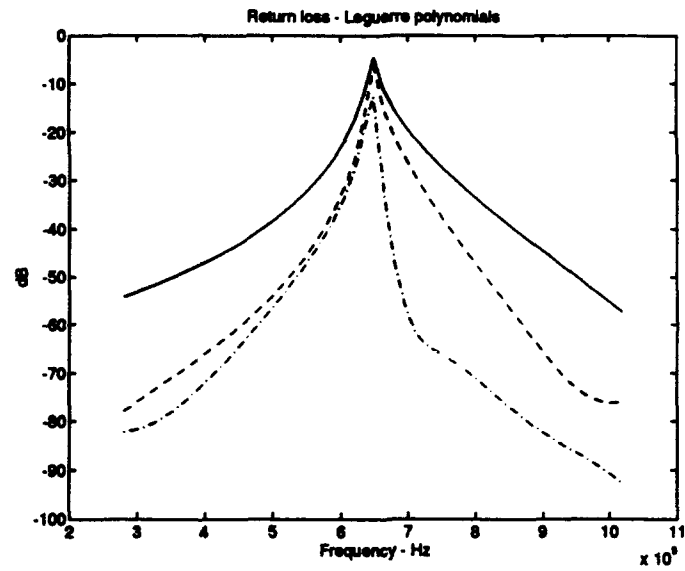


Figure 10: The return loss of the ABC for a TE_{10} mode in a 10.16 by 22.86mm rectangular waveguide. The solid, dashed and dashed dotted lines correspond to two, five and ten Laguerre polynomials used in expansion (74), respectively

3 DISCUSSION

3.1 Algorithm limitations and their applicability to complex problems

The time domain algorithms based on the method of moments and the eigenfunctions expansion are in general less versatile than classical FDTD schemes. One limiting factor is that the structure has to be entirely (for the TEE) or partially (for the PEE) closed (As discussed further, this restriction can be overcome in the PEE if the spherical coordinate system is used). Also because the eigenfunction are available in analytical form only for simple domains, the TEE and PEE are restricted to the analysis of the problems which can be described within such domains. Additionally, the method of moments procedure requires computation of inner products. The numerical cost involved in this process limits the applicability of TEE and PEE to weak and moderate inhomogeneities.

These drawbacks can be alleviated in two ways, one is to replace the eigenfunction expansion with the basis functions with local support. This approach leads to a formulation which may be regarded time domain version of the finite element method. The other possibility is to combine the PEE with a classical FDTD. The hybrid technique will be particularly useful in structures where the inhomogeneities are separated one from the other by homogeneous regions. One problem with a classical FDTD method is that the field from one inhomogeneity to the other has to be propagated, because of the stability requirements the time step size is usually small and if the smallest feature size is also small then the propagation of a field through homogeneous regions requires vast amounts of computer store and time. If the homogeneous regions can be treated with scalar PEE algorithm great savings in computer CPU time and memory resources can be achieved as it often suffices to propagate a few low order modes and additionally the scalar PEE algorithm offers near ultimate speed. The scalar PEE may be regarded here as a fast field propagator. As shown in the numerical tests the hybrid algorithms are also extremely useful to implement the ABC in homogeneous guides so their implementation can offer a significant speed up in the analysis of complex microwave structures.

Examples of practical structures. It should be noted that there many practical complex structures whose geometries are suitable for the application of scalar hybrid PEE-FDTD. For instance most components using rectangular waveguide such as waveguide to coax transition, all kinds of E-plane and dielectric filters, septa, T- and E-H junctions which lead to 3D problems can easily be represented in a combination of PEE and FDTD meshes with 2D homogeneous slices filling most of the volume. In such structures the speed and memory improvement should be significant. Also many 2D structures, including most of planar transmission lines can be described in a hybrid mesh with 1D "slices" located in homogeneous part and FDTD mesh located only in the vicinity of strips, slots etc. The hybrid approach solves here the problem encountered in a classical FDTD where the fine mesh density required in near the small geometrical features has also to cover large homogeneous regions.

3.2 Free space problems

Hybrid PEE-FDTD techniques seem promising for problems of field scattering or radiation in the free space. Here the best approach is to place an object in spherical domain and use the FDTD mesh inside the sphere and the eigenfunction expansion outside. In the PEE part of the algorithm we discretize the space along the r direction and use spherical harmonics for the expansion in the φ and θ directions. In spherical coordinates an open space may be treated as a spherical waveguide [14] which propagates the TE and TM modes. For an open space the wave impedance has the resistive character only if $kr > n$ where n is the order of the spherical Bessel functions. The modes with the resistive impedance radiate while those with the imaginary character of the impedance are confined to the region in the neighborhood of the sources. Hence low order spherical harmonics can be used to describe radiation (scattering) from the sources contained in a sphere of the radius comparable with the shortest wavelength of interest (ie satisfying $kr > n$). Note that the field expansion in the spherical coordinates uses Fourier series in the φ direction so the FDTD and PEE can be easily interfaced through the FFT. There could be a few advantages of this approach. First, we can expect that a hybrid algorithm would require much fewer unknowns than in the FDTD. Second, ABC's can be easier to implement on mode by mode basis as discussed in Section 1.7. A very good performance can be expected. Third, the PEE can be used as a field propagator to allow analysis of fields at larger distances.

3.3 Future developments

Having created the theoretical basis for the algorithms and validated the key techniques, it is possible to define future research directions. There are four topics which seem worth pursuing.

1. A full implementation of a scalar PEE-FDTD algorithm. As shown this algorithm offers near ultimate speed requiring little computer store.
2. Optimisation of the new ABC for highly dispersive structures. The results obtained so far represent the qualitative and quantitative leap in speed, memory and performance compared to the solutions currently used. The emphasis in future research should be placed on the reduction of the reflection at cutoff frequency.
3. The development of the hybrid PEE-FDTD scheme for open space. This can expand the applicability of the methods of moments in time domain.
4. A basic theoretical research in order to develop a suitable set of entire domain expansion functions for 2D inhomogeneous regions. The PEE algorithm currently requires homogeneous slices in order to achieve great speed. With a suitable basis constructed basis, taking into account the inhomogeneities of 2D slices and allowing the arbitrary shapes of the region, the hybrid PEE-FDTD algorithm should give the same versatility as FDTD but at a much greater speed for practically all microwave structures which can be analyzed by current time domain methods.

All four topics are promising from the point of view of numerical cost reduction and can be investigated at the Technical University of Gdańsk.

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FUNCTION EXPANSION ALGORITHMS FOR THE TIME-DOMAIN ANALYSIS OF SHIELDED STRUCTURES SUPPORTING ELECTROMAGNETIC WAVES

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SUMMARY

Series function expansion algorithms of the time-domain analysis of boundary value problems are discussed. Electromagnetic fields inside a structure under investigation are expanded into series of basis functions and the expansion coefficients are found by means of the Galerkin method. The numerical cost of algorithms is discussed and a cost efficient approach is proposed for formulations using sine and cosine expansion functions. Compared with conventional time-domain methods the algorithms described show the time evolution of the expansion coefficients rather than the samples of a physical continuum at discrete nodes.

1. INTRODUCTION

The Fourier transform introduces the equivalence between time and frequency. Therefore each problem involving one of these quantities has two alternative formulations. For many years the frequency-domain formulations have been preferred for the analysis of Maxwell equations. A plethora of frequency-domain numerical methods have been developed and applied to various boundary value problems in electromagnetics. In recent years time-domain techniques have increasingly been gaining an audience. Most research in the area of time-domain algorithms for the modelling of electromagnetic fields was concerned with three versatile and simple methods. These three algorithms are known as the transmission line matrix (TLM), spatial network (SN) and finite difference, time-domain (FDTD) methods. All three techniques are well described in the open literature and therefore we cite here only a few sources.¹⁻⁵ In the TLM and SN methods the structure under investigation is treated as a spatial network of transmission lines and the wave propagation is described by incident and reflected voltage impulses on the mesh lines. In the FDTD method the Maxwell's equations are discretized both in space and time, the derivatives are computed by means of central difference scheme and the fields are evaluated at discrete nodes. Although FDTD and TLM (SN) methods use different concepts and are concerned with different physical quantities, a recent study by Celuch-Marcysiak and Gwarek⁶ shows that each of them can be obtained from the other by a sequence of suitable transformations. Hence, time-domain methods currently used in practice are formally equivalent. Their salient feature is that three-dimensional space is discretized and a mesh is formed. Samples of relevant quantities at mesh points are used to represent a physical continuum. Obviously, while solving complex problems we have always to contend with approximate answers, but nevertheless sampling of the solution in space is only one, not necessarily the most efficient, form of a discrete representation of a physical continuum. For instance in the frequency-domain methods this form of approximation is present in the finite difference technique⁸ and to a certain extent also in the method of lines.⁹ Other algorithms use different representations of fields. One of the most popular frequency-domain techniques consists in field expansion in the series of basis functions. Depending on the algorithm, expansion functions are defined locally or over the entire domain. They can be just mathematical functions or have a physical meaning of, for instance, modes. The expansion coefficients of are most often found using the methods known from functional analysis, such as the method of moments (Galerkin, Ritz), or least squares.¹⁵ Expansion of the fields in series of basis functions underlies such techniques as finite elements, coupled modes, mode-matching, point-matching and iterative eigenfunction expansion,¹⁰⁻¹⁵ to mention only the most powerful.

To the author's best knowledge, the only attempt so far to apply function expansion in the time-domain analysis of shielded microwave structures was published by Nam *et al.*⁷ The expansion function used in that case was obtained using frequency-dependent equations and the algorithm was far more complicated than that of classical time-domain methods.

This introduction shows that, as far as the approximation techniques are concerned, the time-domain methods of the modelling of electromagnetic fields have used so far only a small fragment of a range of choices existing in the frequency domain. In view of that fact the aim of this paper is to look at time-domain algorithms from the point of view of the alternative representation of fields, in order to find formulations which may broaden the range of options available for the time-domain analysis of complex problems of electromagnetics.

2. ANALYSIS

We shall be concerned with the time-domain analysis of shielded structures. Of particular interest are resonators and cylindrical waveguides inhomogeneously loaded with non-dispersive isotropic materials. One possible structure is shown in Figure 1. It is assumed that the bounding walls are perfect electric or magnetic conductors and that the inhomogeneity is described by the relative permittivity, ϵ_r , and permeability, μ_r , both being in general functions of all three space coordinates. Under these assumptions the Maxwell's equations are given by

$$\begin{aligned}\frac{\partial}{\partial t} \mathbf{E} &= \frac{1}{\epsilon_0 \epsilon_r(x,y,z)} \nabla \times \mathbf{H} \\ \frac{\partial}{\partial t} \mathbf{H} &= \frac{-1}{\mu_0 \mu_r(x,y,z)} \nabla \times \mathbf{E}\end{aligned}\quad (1)$$

where ϵ_0 and μ_0 are the permittivity and permeability of the free space.

These equations can be written using the following abbreviated notation

$$\begin{aligned}\frac{\partial}{\partial t} f &= \mathcal{L}_1 g \\ \frac{\partial}{\partial t} g &= \mathcal{L}_2 f\end{aligned}\quad (2)$$

where $\mathcal{L}_1 = 1/\epsilon_0 \epsilon_r(x,y,z) \nabla \times (\cdot)$, $\mathcal{L}_2 = -1/\mu_0 \mu_r(x,y,z) \nabla \times (\cdot)$ and f and g are vector functions representing the electric and magnetic field, respectively. The above notation will be used henceforth.

Replacing the time derivatives with a finite difference equivalents we get the following time-matching equations

$$\begin{aligned}f^n &= f^{n-1} + \Delta t \mathcal{L}_1 g^{n-1/2} \\ g^{n+1/2} &= g^{n-1/2} + \Delta t \mathcal{L}_2 f^n\end{aligned}\quad (3)$$

The unknown functions f, g are now expanded into series of functions.

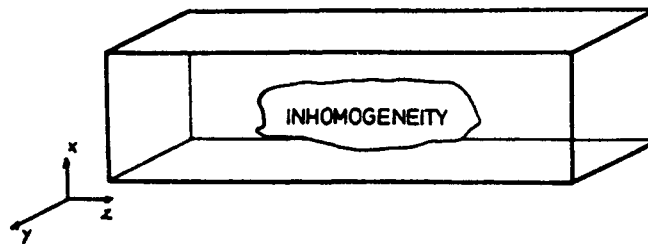


Figure 1. A possible geometry of the problem

$$f^n = \sum a_i^n f_i(x, y, z) \quad g^n = \sum b_i^n g_i(x, y, z) \quad (4)$$

The set of expansion functions is assumed to be complete and the functions are linearly independent. The functions are defined on the entire domain or have local supports but they are in general the time-independent functions of all three spatial variables. Substituting (4) into (3) we get

$$\begin{aligned} \sum a_i^n f_i &= \sum a_i^{n-1} f_i + \Delta t \mathcal{L}_1 \sum b_i^{n-1/2} g_i \\ \sum b_i^{n+1/2} g_i &= \sum b_i^{n-1/2} g_i + \Delta t \mathcal{L}_2 \sum a_i^n f_i \end{aligned} \quad (5)$$

Taking the inner product of (3) with the expansion functions f_i and g_i results in

$$\begin{aligned} \langle f^n, f_i \rangle &= \langle f^{n-1}, f_i \rangle + \Delta t \langle \mathcal{L}_1 g^{n-1/2}, f_i \rangle \\ \langle g^{n+1/2}, g_i \rangle &= \langle g^{n-1/2}, g_i \rangle + \Delta t \langle \mathcal{L}_2 f^n, g_i \rangle \end{aligned} \quad (6)$$

Using (5) the above equations can be cast into the following matrix form

$$\begin{aligned} \mathbf{a}^n &= \mathbf{a}^{n-1} + \Delta t \mathbf{C}^{-1} \mathbf{A} \mathbf{b}^{n-1/2} \\ \mathbf{b}^{n+1/2} &= \mathbf{b}^{n-1/2} + \Delta t \mathbf{D}^{-1} \mathbf{B} \mathbf{a}^n \end{aligned} \quad (7)$$

where \mathbf{a} and \mathbf{b} are the vectors containing expansion coefficients and \mathbf{A} , \mathbf{B} , \mathbf{C} , \mathbf{D} are matrices with elements given by the following inner products

$$\begin{aligned} A_{ij} &= \langle \mathcal{L}_1 g_j, f_i \rangle & b_{ij} &= \langle \mathcal{L}_2 f_j, g_i \rangle \\ C_{ij} &= \langle f_j, f_i \rangle & D_{ij} &= \langle g_j, g_i \rangle \end{aligned} \quad (8)$$

All matrices defined above are in general dense. If the expansion functions are orthonormal then \mathbf{C} and \mathbf{D} are identity matrices and (7) becomes

$$\begin{aligned} \mathbf{a}^n &= \mathbf{a}^{n-1} + \Delta t \mathbf{A} \mathbf{b}^{n-1/2} \\ \mathbf{b}^{n+1/2} &= \mathbf{b}^{n-1/2} + \Delta t \mathbf{B} \mathbf{a}^n \end{aligned} \quad (9)$$

So far we have presented the algorithms in which the time is discretized and the function expansion is done in three dimensions. We shall call them total expansion algorithms. Another version of the expansion algorithm is obtained if the discretization is in time and one selected coordinate and the expansion is done with respect to two remaining coordinates. This approach combines the FDTD method with the expansion algorithms described above. The space is sliced into subdomains (Figure 2) and the fields are expanded on each subdomain (slice) into series of

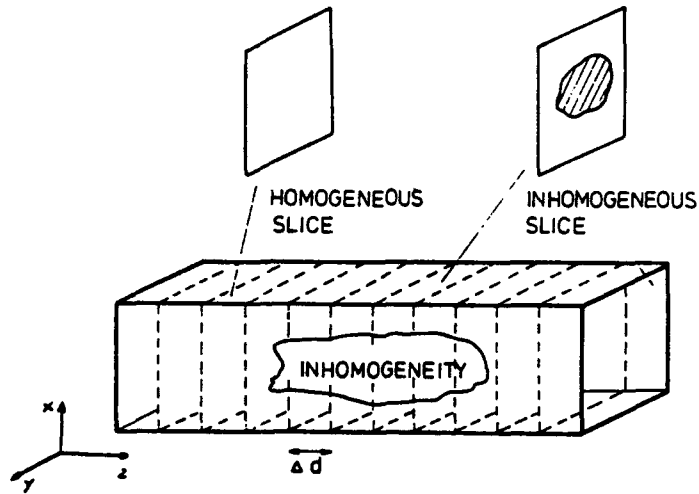


Figure 2. Division of the geometry for the partial expansion algorithms

expansion functions. This type of expansion we shall call partial. To obtain the time-marching equations for such a case we have to introduce the finite difference scheme for the calculation of the space derivatives with respect to the discretized variable. Suppose the structure was divided into K slices in the z -direction and the slices are uniformly spaced by the distance Δd . To enable the application of the central finite difference scheme for the calculation of the derivatives in the z -direction we use the technique used in the FDTD method. In this technique² different field components are defined on two meshes, each off by half the space step from the other. This arrangement is known as Yee's mesh. In the present context Yee's mesh is given in one spatial dimension, which means that relevant field components are defined on the slices that are off by half the space step. More precisely the E_x^k, E_y^k, H_z^k are given at $z = k\Delta d$ and H_x^k, H_y^k, E_z^k are defined for $z = (k + 1/2)\Delta d$. Bearing this convention in mind we expand fields at a suitably situated slice according to

$$f_k^* = \sum a_{ik}^* f_i(x, y) \quad g_k^* = \sum b_{ik}^* g_i(x, y) \quad k = 1, \dots, K \quad (10)$$

The derivatives in the z -direction are approximated by

$$\frac{\partial}{\partial z} \psi_{k+1/2} \approx \frac{\psi_{k+1} - \psi_k}{\Delta d} \quad (11)$$

Calculation of the z -derivatives involves operations on the functions defined on the adjacent slices. Therefore, instead of equations (2) we get

$$\begin{aligned} \frac{\partial}{\partial t} f_k &= \mathcal{L}_{1t}^k g_k + \mathcal{L}_{1z}^k (g_{k+1} - g_k) \\ \frac{\partial}{\partial t} g_k &= \mathcal{L}_{2t}^k f_k + \mathcal{L}_{2z}^k (f_k - f_{k-1}) \end{aligned} \quad (12)$$

Where we have split operators \mathcal{L}_1 and \mathcal{L}_2 into transverse and z - part according to

$$\begin{aligned} \mathcal{L}_{1t}^k &= \frac{1}{\epsilon_0 \epsilon_r^k(x, y)} \nabla_t \times (\cdot) & \mathcal{L}_{1z}^k &= \frac{1}{\epsilon_0 \epsilon_r^k(x, y) \Delta d} \mathbf{i}_z \times (\cdot) \\ \mathcal{L}_{2t}^k &= \frac{-1}{\mu_0 \mu_r^k(x, y)} \nabla_t \times (\cdot) & \mathcal{L}_{2z}^k &= \frac{-1}{\mu_0 \mu_r^k(x, y) \Delta d} \mathbf{i}_z \times (\cdot) \end{aligned} \quad (13)$$

In the above equations by \mathbf{i}_z we have denoted a unit vector in the z -direction.

Replacing time derivatives by the finite difference scheme, expanding functions in (12) and taking the inner products for each slice we arrive at the set of equations similar to (7) with the block-diagonal coefficient matrices given by

$$\begin{aligned} \mathbf{A} &= \text{qdiag} [\mathbf{A}'^k, \mathbf{A}''^k] & \mathbf{B} &= \text{qdiag} [\mathbf{B}'^k, \mathbf{B}''^k] \\ \mathbf{C} &= \text{qdiag} [\mathbf{C}^k] & \mathbf{D} &= \text{qdiag} [\mathbf{D}^k] \end{aligned} \quad (14)$$

The elements of the submatrices are given

$$\begin{aligned} \mathbf{A}_i'^k &= \langle (\mathcal{L}_{1t}^k - \mathcal{L}_{1z}^k) g_{ik}, f_{ik} \rangle & \mathbf{A}_i''^k &= \langle \mathcal{L}_{1z}^k g_{i, k+1}, f_{ik} \rangle \\ \mathbf{B}_i''^k &= \langle (\mathcal{L}_{2t}^k + \mathcal{L}_{2z}^k) f_{ik}, g_{ik} \rangle & \mathbf{B}_i'^k &= -\langle \mathcal{L}_{2z}^k f_{i, k-1}, g_{ik} \rangle \\ \mathbf{C}_i^k &= \langle f_{ik}, f_{ik} \rangle \\ \mathbf{D}_i^k &= \langle g_{ik}, g_{ik} \rangle \end{aligned} \quad (15)$$

For orthonormal basis functions matrices \mathbf{C} and \mathbf{D} become identity matrices and we get again (9). Thus both total and partial time-domain expansion algorithms are formally described by the same set of equations (7) or (9). However, one important difference between the total and partial

expansion algorithms is that in the former the matrices (8) are in general dense while in the latter the matrices (15) are always quasi-diagonal.

Compared with the FDTD method the expansion algorithms show the time evolution of the expansion coefficients rather than field components at nodes. Obviously the expansion algorithms have to use timestep small enough to prevent the instability. At this point it is not possible to give one stability criterion for the algorithms discussed as it depends on the choice of the expansion functions.

3. BASIS FUNCTIONS

Before we discuss the numerical cost involved in the time domain expansion algorithms we shall consider the choice of expansion functions. As we indicated earlier, in both total and partial expansion algorithms individual basis functions can have local support or be defined in the entire domain or subdomain (slice). The advantage of the first approach is that it increases the sparsity of the matrices. On the other hand choosing the basis functions which have the space distribution of the relevant field components of modes in the corresponding *homogeneous* problem, we obtain the following advantages

- (1) expansion functions satisfy the boundary conditions
- (2) owing to the orthogonality of mode functions in homogeneous problems, the inner products at homogeneous slices (Figure 2) in the partial expansion algorithms result in diagonal submatrices A^k , A'^k , B^k , B'^k
- (3) the time-marching algorithms receive a new physical interpretation. They can now be viewed as the equations describing mode coupling due to inhomogeneity. This interpretation allows a straightforward investigation of mode interaction in loaded guides and resonators
- (4) for small inhomogeneities only a few expansion functions will be sufficient to approximate field distribution with good accuracy

A suitable choice for the time-independent basis functions which have the distribution of modes of a homogeneous structure are the eigenfunctions of the Laplace operator. The detailed discussion of the choice of the complete basis for arbitrarily shaped domains and the relation between the eigenfunctions of Laplace operator and modes of a homogeneous structure is given in Reference 15. This discussion shows that for the total expansion algorithms and arbitrarily shaped region closed by the perfect electric conductor S we may use the following representation of fields

$$\begin{aligned} \mathbf{E} &= \sum (a_i \mathbf{e}_i + a'_i \mathbf{e}'_i) \\ \mathbf{H} &= \sum (b_i \mathbf{h}_i + b'_i \mathbf{h}'_i) \end{aligned} \quad (16)$$

where \mathbf{e}_i and \mathbf{h}_i are solenoidal eigenfunctions of a vector Laplace operator

$$\nabla^2 \mathbf{e} + \lambda \mathbf{e} = 0 \quad \nabla^2 \mathbf{h} + \lambda \mathbf{h} = 0 \quad (17)$$

with suitable boundary conditions, and \mathbf{e}'_i and \mathbf{h}'_i are potential functions obtained from eigenfunctions of a scalar Laplace operator

$$\nabla^2 \phi + \lambda \phi = 0 \quad (18)$$

with Dirichlet (for the derivation of \mathbf{e}'_i) and Neumann (for \mathbf{h}'_i) boundary conditions. Here functions \mathbf{e}_i and \mathbf{h}_i correspond directly to the modes of a homogeneous resonator. In the case of the partial eigenfunction expansion a suitable form of representation involving time-independent basis functions is

$$\begin{aligned} \mathbf{E} &= \sum (a_{xi} \mathbf{e}_{xi} + a_{ni} \mathbf{e}_{ni} + a'_{ii} \mathbf{e}'_{ii}) \\ \mathbf{H} &= \sum (b_{xi} \mathbf{h}_{xi} + b_{ni} \mathbf{h}_{ni} + b'_{ii} \mathbf{h}'_{ii}) \end{aligned} \quad (19)$$

Subscripts z and t refer to z and transverse component, respectively. Functions e_{zi} , h_{zi} , e'_{ti} are obtained from the eigenfunctions of a scalar Laplace operator with Dirichlet boundary conditions and functions h_{zt} , e_{zt} , h'_{ti} are derived from the eigenfunctions of a scalar Laplace operator with Neumann boundary conditions. In terms of TE and TM modes, functions e_{zi} , h_{zi} , e'_{ti} contribute to TM modes in a homogeneous guide and h_{zt} , e_{zt} , h'_{ti} produce TE fields.

For simple regions, S , it may be also possible to expand each field component separately using the eigenfunctions of a scalar Laplace operator with mixed Dirichlet/Neumann boundary conditions.

4. NUMERICAL COSTS OF THE TIME-DOMAIN EXPANSION ALGORITHMS

One drawback of the expansion algorithms presented in the previous section is that they may lead to higher numerical cost than FDTD and TLM. The inner products appearing in (8) and (15) are independent of time and can be stored in look-up tables. If the cost of the calculation of inner products is neglected in the algorithms then the cost of one timestep of the algorithms is determined by the cost of matrix multiplication. Depending on the basis functions used (local support versus entire domain) the overall cost may vary considerably. Generally speaking, assuming that expansion is done using L eigenfunctions, the cost of one timestep is of order $O(L^2)$. If the matrices are sparse the cost is lower. In the FDTD and TLM method with N nodes, the numerical cost is of order $O(N)$. Consequently, expansion techniques are comparable in terms of numerical cost and memory to classical time-domain algorithms when $L^2 \sim N$. This condition will easily be fulfilled in slightly and moderately perturbed homogeneous structures when the basis functions have the space distribution of the relevant field components of modes in the corresponding homogeneous problem. A similar conclusion can be derived regarding memory requirements.

At this point it is important to note that a very efficient implementation of the expansion algorithms may be obtained if the expansion functions are sine and cosines. Let us consider the total expansion algorithm described by (9). Equations (6) imply that at each step one evaluates the inner products $\langle \mathcal{L}_1 g^{n-1/2}, f_i \rangle$ and $\langle \mathcal{L}_2 f^n, g_i \rangle$ and these inner products are used to update expansion coefficients. For sine and cosine functions the inner product for all testing functions can be computed in a very efficient way using the technique described in Reference 14. In this technique the *all* inner products are computed in one step in a sequence of inverse and forward FFTs. In a nutshell the procedure is

- using *inverse* 3-D FFT and $h^{n-1/2}$ and a^n calculate $g^{n-1/2}$, f^n and their spatial derivatives
- Compute functions $\mathcal{L}_1 g^{n-1/2}$ and $\mathcal{L}_2 f^n$
- using *forward* 3-D FFT compute all inner products $\langle \mathcal{L}_1 g^{n-1/2}, f_i \rangle$ and $\langle \mathcal{L}_2 f^n, g_i \rangle$

The numerical cost of such computations is relatively low and there is no need to create look-up matrices A and B. As a result the time-domain algorithms can be implemented using very little computer storage and with a speed comparable to that of the corresponding FDTD or TLM methods.

It is beyond the scope of this paper to discuss in detail the numerical implementations of the algorithms presented herein. However, both total and partial expansion algorithms have been implemented and tested by the author for case of the rectangular resonators containing dielectric slabs. The eigenfunctions of the Laplace operator with Dirichlet or Neumann boundary conditions were used as the expansion functions and the inner products were calculated using fast Fourier transform approach described in the above section. The algorithms have been found stable. Some numerical results for the expansion algorithms with sine and cosine expansion functions are given in Table I and Reference 16. Table I compares the results obtained for fundamental mode in a rectangular resonator shown in Figure 3 using the total and partial expansions algorithms with the data FDTD published in Reference 5 and rigorous methods. It can be noted that the results in the table obtained with the expansion algorithms are in a very good agreement with the reference values which confirm the validity of the analysis proposed in this paper.

5. CONCLUSIONS

Algorithms of the time-domain analysis of inhomogeneously loaded microwave structures have been described. The methods proposed are based on the expansion of fields into complete series

Table I. Comparison of the results for the normalized resonant frequencies Δ/λ obtained using expansion algorithms with the published data⁵ for the rectangular resonator shown in Figure 3

	TRM	Partial expansion	Total expansion	FDTD ⁵
$w = 0$	0.07511 (exact)	0.07502	0.07511	0.0750
$w = 2\Delta$	0.0522	0.05253	0.05153	0.0517
$w = 4\Delta$	0.0445	0.04456	0.04433	0.0442

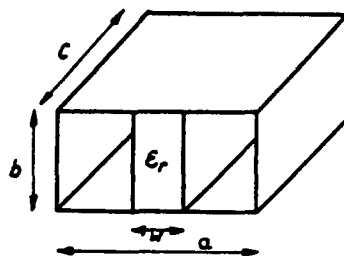


Figure 3. The geometry of the problem used in the numerical test ($a = 12\Delta$, $b = 6\Delta$, $c = 8\Delta$, $\epsilon_r = 3.75$)

of basis functions. The resulting equations show the time evolution of the expansion coefficients. With a suitable choice of basis functions this feature allows one to investigate propagation of separate modes and their mutual interactions.

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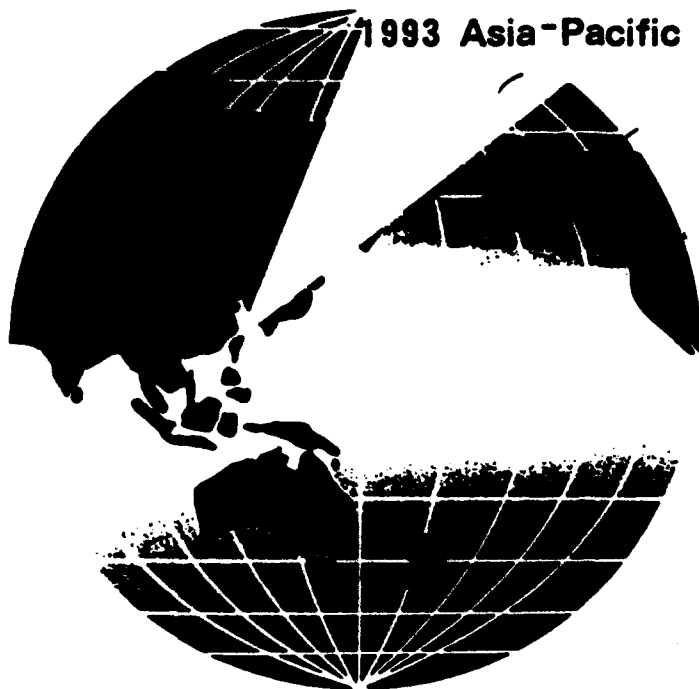
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Stability of the Time Domain Total Eigenfunction Expansion Algorithm

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ABSTRACT

The paper presents the derivation of the stability condition for the total eigenfunction expansion algorithm for the solution of Maxwell's equations. The algorithm uses the method of moment solution for space and leap-frog differencing scheme for time. The stability condition of the algorithm is derived by investigating the properties of operators in suitably defined Hilbert spaces. The approach is general and can be used for other iterative algorithms.

1. INTRODUCTION

At present there are two algorithms, namely the TLM and FD-TD [1],[2], which dominate the arena of time domain solution of Maxwell's equations. In both methods the space is discretized and derivatives are approximated by finite differences. If, however, the sampling of at the mesh nodes is replaced by the series expansion of fields and the expansion coefficients are found using the method of moment, new algorithms can be created. Two such algorithms have been recently proposed by the author of this contribution [3], [4].

A simplest time domain algorithm based on the concept briefly described above is called a total eigenfunction expansion (TEE) [3], [4]. Let us consider a set of coupled differential equations reflecting the form of Maxwell equations

$$\begin{aligned}\frac{\partial}{\partial t} f &= L_1 g \\ \frac{\partial}{\partial t} g &= L_2 f\end{aligned}\quad (1)$$

where $L_1 = \frac{1}{\epsilon_0 \epsilon_r(x,y,z)} \nabla \times (\cdot)$, $L_2 = \frac{-1}{\mu_0 \mu_r(x,y,z)} \nabla \times (\cdot)$ and f and g are vector functions representing the electric and magnetic field, respectively. Instead of discretizing the fields, equations (1) are solved by means of the method of moments and only time derivatives are calculated using the finite differencing scheme. Replacing the time derivatives with finite difference equivalents we get the following time marching equations

$$\begin{aligned}f^n &= f^{n-1} + \Delta t L_1 g^{n-1/2} \\ g^{n+1/2} &= g^{n-1/2} + \Delta t L_2 f^n\end{aligned}\quad (2)$$

The unknown functions f, g are now expanded into series of functions.

$$f^n = \sum a_i^n f_i(x, y, z) \quad g^n = \sum b_i^n g_i(x, y, z) \quad (3)$$

Expansion functions are defined on the entire domain. A sensible choice for the electromagnetic fields are the eigenfunctions of Laplace operator with suitable boundary conditions. Applying a standard method of moment procedure by taking the inner product of (2) with the expansion functions f_i and g_i we get

$$\begin{aligned}
\langle f^n, f_i \rangle &= \langle f^{n-1}, f_i \rangle \\
+\Delta t \langle L_1 g^{n-1/2}, f_i \rangle \\
\langle g^{n+1/2}, g_i \rangle &= \langle g^{n-1/2}, g_i \rangle \\
+ \Delta t \langle L_2 f^n, g_i \rangle &(4)
\end{aligned}$$

The above equations can be cast into the following matrix form

$$\begin{aligned}
\mathbf{a}^n &= \mathbf{a}^{n-1} + \Delta t \mathbf{C}^{-1} \mathbf{A} \mathbf{b}^{n-1/2} \\
\mathbf{b}^{n+1/2} &= \mathbf{b}^{n-1/2} + \Delta t \mathbf{D}^{-1} \mathbf{B} \mathbf{a}^n \quad (5)
\end{aligned}$$

where \mathbf{a} and \mathbf{b} are the vectors containing expansion coefficients and \mathbf{A} , \mathbf{B} , \mathbf{C} , \mathbf{D} are matrices with elements given by the following inner products

$$\begin{aligned}
A_{ij} &= \langle L_1 g_j, f_i \rangle & B_{ij} &= \langle L_2 f_j, g_i \rangle \\
C_{ij} &= \langle f_j, f_i \rangle & D_{ij} &= \langle g_j, g_i \rangle \quad (6)
\end{aligned}$$

2. STABILITY CONDITION

The algorithm described above was proven to provide an accurate solution for inhomogeneously loaded rectangular resonator [3], [4]. However, during the numerical tests it was observed that the maximal time step size depends on the number of functions used in the expansion. This time step size is a key factor which allows one to derive the stability criterion for the algorithm. For the FD-TD and TLM method the stability criterion is known as a Courant conditions, but the stability of TEE algorithm has never been examined yet. This contribution will present the results of the stability analysis of the TEE algorithm

Presently we shall derive the stability criterion for the total expansion using trigonometric series expansion. Before deriving the stability criterion let us present problem (1) in the form of a hyperbolic equation. Taking the time derivative of the first equation and applying operator L_1 to the second equations we obtain.

$$\frac{\partial^2}{\partial t^2} f = L_1 L_2 f \quad (7)$$

Putting $L = -L_1 L_2$ we get

$$\frac{\partial^2}{\partial t^2} f + Lf = 0 \quad (8)$$

L is an elliptic differential operator with positive coefficients so (8) is hyperbolic differential equation. Stability of the differencing schemes can be studied using the methods of functional analysis. In [5] such an approach was used for the case of classical finite difference representation of L . The theorems used in that case are also applicable to this method. To investigate the stability time marching algorithms for the hyperbolic equations it is useful to present a problem in a canonical form

$$(I + \Delta^2 t R) \frac{\partial^2}{\partial t^2} f + A f = 0 \quad (9)$$

Where I is the identity operator.

The time marching algorithm for the above problem is stable if the following conditions are fulfilled [5]:

$$A = A^* > 0, \quad R = R^* > 0 \quad (10)$$

$$R - 0.5A \geq 0 \quad (11)$$

In other words for the time marching algorithm to be stable it is sufficient that both operators A and R are self adjoint and positive and additionally the operator $R - 0.5A$ is nonnegative. The canonical form (9) is obtained from (8) by simply multiplying it by 2 and writing the result as

$$(I + \frac{\Delta^2 t}{\Delta^2 t} I) \frac{\partial^2}{\partial t^2} f + 2L f = 0 \quad (12)$$

Comparing (12) with (9) we get $R = I/\Delta^2 t$ and $A = 2L$. It can readily be verified that operator L is symmetric and positive. It suffices to verify the condition (11). This condition is fulfilled when

$$\| \frac{I}{\Delta^2 t} \| \geq \| L \| \quad (13)$$

or

$$\Delta t \leq \frac{1}{\| L \|} \quad (14)$$

It is seen that the stability depends on the norm of the operator L . The norm of the operator depends on the space it acts in. Let us estimate the norm of the operator L in a finite dimensional linear space spanned by trigonometric functions.

Suppose that the inhomogeneity is located inside a cubical resonator with the dimensions $l \times l \times l$. The expansion functions are normalized products of sines and cosines of the form

$$\sin \frac{i\pi\xi}{l} \text{ or } \cos \frac{k\pi\xi}{l} \quad i, k \leq N_M \quad (15)$$

Let \mathcal{D} denote the domain of the original problem given by equations (1). The basis functions (15) span a finite dimensional space $\mathcal{H}_{N_M} \subset \mathcal{D}$ in which the approximate solution is sought for. In such constructed space we calculate the upper bound of the norm of operator $\|L\|$. Note that $\|L\| \leq \|L_m\|$. Where

$$L_m = (\epsilon_0 \mu_0 \epsilon_{\min} \mu_{\min})^{-1} \nabla \times \nabla \times (\cdot) \quad (16)$$

and

$$\begin{aligned} \epsilon_{\min} &= \inf \epsilon_r(x, y, z), \\ \mu_{\min} &= \inf \mu_r(x, y, z) \quad x, y, z \in \Omega \end{aligned} \quad (17)$$

The norm of operator L in \mathcal{H}_{N_M} can now readily be found

$$\|L\| \leq \|L_m\| \leq v_{\max} \frac{N_M \pi \sqrt{3}}{l} \quad (18)$$

where $v_{\max} = (\epsilon_0 \mu_0 \epsilon_{\min} \mu_{\min})^{-1/2}$ is the maximal velocity which a plane wave attains in the medium filling the structure. Using the above estimation we get the following stability condition

$$\Delta t \leq \frac{l}{v_{\max} N_M \pi \sqrt{3}} \quad (19)$$

If a Ω is a perpendicular parallelepiped with the dimensions $a \times b \times l$ and the upper bound for i, l, m in the trigonometric expansion functions is K_M, L_M, N_M then the condition (19) becomes

$$\Delta t \leq \frac{1}{v_{\max} \pi \sqrt{(\frac{K_M}{a})^2 + (\frac{L_M}{b})^2 + (\frac{N_M}{l})^2}} \quad (20)$$

3. CONCLUSIONS

The derivation of the stability condition for the total eigenfunction expansion algorithm for the solution of Maxwell's equations is presented. The stability condition of the algorithm is derived using the methods of functional analysis. The approach is general and can be used for other iterative algorithms.

4. ACKNOWLEDGMENT

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SECOND INTERNATIONAL WORKSHOP

on

Discrete Time Domain Modelling of Electromagnetic Fields and Networks



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In collaboration with the
MTT Technical Committee on Field Theory
(MTT-15)

October 28 and 29, 1993

Hotel Ambassador
Berlin, Germany

Friday, October 29, 1993:

Session B2 (Chairmen: L.P.B. Katehi, L. Felsen)

- | | | |
|-------|-------------------------------------------------------------------------------------------------------------------------|------------------------------------|
| 15:00 | Simulation of Electromagnetic Fields in Nonlinear and Photonic Waveguiding Structures | D. Jaeger |
| 15:10 | Derivation of Stability Condition for the Time Domain Method of Moments Algorithms Using Functional Analysis Approach | M. Mrozowski |
| 15:20 | Convergence Criteria for Maxemol - a Numerical Scheme for the Solution of Maxwell's Equations Using the Method of Lines | W.B. Fu, R.A.C. Metaxas |
| 15:30 | Broadband Simulation of Open Waveguide Boundaries within Large Frequency Ranges | M. Dohlus, P. Thoma,
T. Weiland |
| 15:40 | On the Geometrical Structure of Network Equations | St. Paul |
| 15:50 | Further Late Contributions | |
| 16:00 | Concluding Session: open forum, panel discussion, approximately finished by 17:00 | |

Derivation of Stability Condition for the Time Domain Method of Moments Algorithms Using Functional Analysis Approach

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ABSTRACT

This contribution presents the derivation of the stability condition for time domain method of moment for linear hyperbolic differential equations. The algorithm uses the method of moment approach for space variables and finite difference scheme for time. The stability condition of the algorithm is derived by investigating the properties of operators in suitably defined Hilbert spaces. The method discussed in this contribution has been developed in context of the time domain analysis of Maxwell's equations but the approach is general and can be used for other explicit algorithms.

INTRODUCTION

Functional analysis is one of the most powerful tools of the theoretical investigation of the basic properties of numerical methods. The methods of functional analysis are commonly used in the mathematical physics, numerical mathematics and computer science but seldom in engineering. At the same time the engineering creates demand for new more efficient numerical methods which would provide a sufficiently accurate solution as fast as possible. This results in the constant improvements of published algorithms by researchers who adapt them to their particular needs without investigation of the properties of modified algorithms. For instance, explicit algorithms for the solution of initial value problems have recently received much attention among researchers involved in the numerical analysis of electromagnetic fields. Two methods belonging to this class, known as finite difference-time

domain (FDTD) and transmission line matrix (TLM) algorithms have intensively been developed in the last decade. Their salient feature is that electromagnetic field is analyzed in the time domain and the samples of relevant physical quantities at nodes located at the discrete points in space are used to represent a physical continuum. These two methods are constantly being improved. The improvements include the application of graded meshes or non orthogonal cells, application of local approximations or extension of the basic algorithms to the new class of materials such as ferrites or dispersive media. Also new concepts of space representation of fields have been introduced. The sampling at discrete points can be replaced by the expansion into the series of basis functions and the expansion coefficients found by the method of moments procedure.

Recognizing the progress achieved in the recent years in the time domain analysis of electromagnetic fields, it should be noted, that the explicit algorithms underlying these methods are not unconditionally stable and the improvements introduced to algorithms affect their stability. In this contribution we shall present how the effects of the algorithm modifications can be investigated using the functional analysis.

STABILITY ANALYSIS OF EXPLICIT TIME DOMAIN ALGORITHMS

Let us consider a hyperbolic differential equation

$$\frac{\partial^2}{\partial t^2} f + Lf = 0 \quad (1)$$

where L is a linear elliptic differential operator with positive coefficients. The hyperbolic equation of this type, supplemented by conditions at $t = 0$ can be solved for $t > 0$ using a classical finite difference explicit algorithm. For L being a Laplacian the stability criterion for the algorithm is known as the Courant condition. For other operators it is convenient to use the methods of functional analysis. In [2] such an approach was used for the case of finite difference representation of L . The theorems used in that case are general so it is very instructive to show how they can be applied for other explicit algorithms.

To investigate the stability of a time marching algorithms for the hyperbolic equations it is useful to present a problem in a canonical form

$$(I + \Delta^2 t R) \frac{\partial^2}{\partial t^2} f + A f = 0 \quad (2)$$

Where I is the identity operator.

The time marching algorithm for the above problem is stable if the following conditions are fulfilled [2]:

$$A = A^* > 0, \quad R = R^* > 0 \quad (3)$$

$$R - 0.5A \geq 0 \quad (4)$$

In other words for the explicit algorithm to be stable it is sufficient that both operators A and R be self adjoint and positive and additionally the operator $R - 0.5A$ be nonnegative.

A linear operator F defined in a Hilbert space $(H, \langle \cdot, \cdot \rangle)$ is self adjoint if for any $x, y \in H$

$$\langle Fx, y \rangle = \langle x, Fy \rangle^* \quad (5)$$

An operator F is positive $F > 0$ (or nonnegative $F \geq 0$) when for all $x \in H, x \neq 0$ we have

$$\langle Fx, x \rangle > 0 \quad \text{or} \quad \langle Fx, x \rangle \geq 0 \quad (6)$$

The canonical form (2) is obtained from (1) by simply multiplying it by 2 and writing the result as

$$(I + \frac{\Delta^2 t}{\Delta^2 t} I) \frac{\partial^2}{\partial t^2} f + 2L f = 0 \quad (7)$$

Comparing (7) with (2) we get $R = I/\Delta^2 t$ and $A = 2L$

If operator L is symmetric and positive than the stability condition is

$$\| \frac{I}{\Delta^2 t} \| \geq \| L \| \quad (8)$$

or

$$\Delta t \leq \frac{1}{\sqrt{\| L \|}} \quad (9)$$

It is seen that the stability depends on the norm of the operator L . The norm of the operator depends on the space it acts in.

STABILITY ANALYSIS FOR THE TIME DOMAIN METHOD OF MOMENTS

Let us consider a one dimensional second order equation

$$\frac{\partial^2}{\partial t^2} f - b(x) \frac{\partial^2}{\partial x^2} f = 0 \quad (10)$$

$$f(x, t_0) = f_0(x), \quad f(x=0) = f(x=a) = 0 \quad (11)$$

where $b(x) > 0$ is a time independent continuous function of x , Instead of using the finite difference representation of $\frac{\partial^2}{\partial x^2}$ let us combine the explicit algorithm with the method of moments. To this end we will use the finite differences for the approximation of time derivatives, expand the function $f(x)$ into series of sines

$$f(x) = \sum c_i \sin(i\pi x/a) \quad (12)$$

and use the inner product

$$\langle u, v \rangle = \int_0^a uv \, dx \quad (13)$$

to find the expansion coefficient at any instance of time. (A detailed derivation of the time domain method of moments for Maxwell's equations can be found in [1])

It can easily be verified that operator

$$\mathbf{L} = -b(x) \frac{\partial^2}{\partial x^2} \quad (14)$$

is positive and self adjoint. This case was considered previously so we may conclude that the algorithm is stable if

$$\Delta t \leq \frac{1}{\sqrt{\|\mathbf{L}\|}} \quad (15)$$

At this point it is necessary to estimate the norm of \mathbf{L} . The problem is defined in the Hilbert space spanned over sine functions. The norm of \mathbf{L} in such a space can be estimated as follows

$$\|\mathbf{L}\| \leq \|\mathbf{L}_M\| = \frac{\langle \mathbf{L}_M x, x \rangle}{\|x\|} = b_{max} \frac{(i\pi)^2}{a^2} \quad (16)$$

where b_{max} is the maximal value of $b(x)$ over the interval $0 < x < a$.

We may conclude that the explicit algorithm combined with the method of moment with sine series will be stable if the time step is chosen such that

$$\Delta t \leq \frac{a}{i\pi\sqrt{b_{max}}} \quad (17)$$

Note that maximal time step is inversely proportional to number of basis functions.

Obviously, the same procedure can be applied to other types of expansion functions, including for instance finite elements. It is important to note however that the time step in the explicit algorithm depends not only on the operator (equation) solved but also on the way the approximation of space is constructed.

CONCLUSIONS

The application of the functional analysis to the investigation of the stability of time domain algorithms has been presented. The method can easily be applied to the investigation of the properties of novel time domain schemes for Maxwell's equations such as the ones proposed in [1].

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A Hybrid PEE-FDTD Algorithm for Accelerated Time Domain Analysis of Electromagnetic Waves in Shielded Structures

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ABSTRACT: A new algorithm for the time domain analysis of electromagnetic waves in shielded structures is presented. The algorithm combines the FDTD with a recently developed partial eigenfunction expansion (PEE) scheme to obtain acceleration in numerical calculation and savings in computer memory. An example of the application of the algorithm is presented showing an overall speed improvement.

INTRODUCTION

Time domain techniques are gaining increased popularity in the analysis of electromagnetic waves because of their ability to treat complicated geometries over a wide frequency range. Because the most popular time domain algorithms are explicit, the stability of the algorithm puts a restriction on the maximum allowable time step. Additionally, to obtain fine resolution of fields near singularities, mesh size is reduced thereby increasing the computer storage. The computation time and memory requirements are therefore critical parameters for time domain algorithms. Because of that some research effort has recently been devoted to the acceleration of the traditional methods by the application of the signal processing [2] techniques, graded mesh schemes [1] or elimination of redundant field components [3].

This contribution presents a new algorithm for shielded structures which consists in the replacement of the FDTD calculation in homogeneous shielded subregions by eigenfunction expansion. The eigenfunction expansion schemes in time domain proposed in [4] rely on the expansion of the unknown functions of selected space variables into series of basis functions and application of method of moment procedure to find the expansion coefficients. One version of the algorithm called the Partial Eigenfunction Expansion (PEE), is obtained if the function expansion is done with respect to two selected space coordinates while the third spatial coordinate and time are discretized in a way analogical to the finite difference scheme. By combining such an approach with a classical FDTD algorithm an improvement in speed can be obtained for an important class of shielded structures.

FORMULATION

As the FDTD is a well known technique, let us begin with the presentation of the second scheme, namely the Partial Eigenfunction Expansion (PEE). Consider a dielectric inhomogeneity located in a rectangular waveguide (fig.1). In the PEE the computational space is sliced into subdomains and the fields are expanded on each subdomain (slice) into series of expansion functions which depend only on transverse coordinates and fulfill the boundary conditions on the guide periphery. The function expansion is done in two dimensions for each slice separately while the variations in the third spatial dimension and time are handled using the finite difference approximations. Suppose the structure was divided into K slices in the z direction and the slices are uniformly spaced by the distance Δd . Using the finite difference approximation of derivatives in the z directions the Maxwell's equations can be written in the following operator form

$$\begin{aligned}\frac{\partial}{\partial t} f_k &= L_{1t}^k g_k + L_{1z}^k (g_{k+1} - g_k) \\ \frac{\partial}{\partial t} g_k &= L_{2t}^k f_k + L_{2z}^k (f_k - f_{k-1})\end{aligned}\quad (1)$$

where f_k and g_k are vector functions representing the electric and magnetic field at the k -th slice and

$$\begin{aligned} L_{1t}^k &= \frac{1}{\epsilon_0 \epsilon_r^k(x, y)} \nabla_t \times (\cdot) & L_{1z}^k &= \frac{1}{\epsilon_0 \epsilon_r^k(x, y) \Delta d} \hat{z} \times (\cdot) \\ L_{2t}^k &= \frac{-1}{\mu_0 \mu_r^k(x, y)} \nabla_t \times (\cdot) & L_{2z}^k &= \frac{-1}{\mu_0 \mu_r^k(x, y) \Delta d} \hat{z} \times (\cdot) \end{aligned} \quad (2)$$

In the above equations by \hat{z} we have denoted a unit vector in the z direction.

The fields are now expanded separately on each slice according to

$$f_k(t) = \sum_i a_{i,k}(t) f_{i,k}(x, y) \quad g_k = \sum_i b_{i,k}(t) g_{i,k}(x, y) \quad k = 1 \dots K \quad (3)$$

where $a_{i,k}, b_{i,k}$ are the expansion coefficients (time dependent) and $f_{i,k}(x, y), g_{i,k}(x, y)$ are the basis functions. The next step is to introduce the expansion (3) into (1) and replace time derivatives by finite difference formulas. This results in equations in which the only unknowns, for a fixed time instant, are the expansion coefficients at all slices of the structure. To evaluate the expansion coefficients we take the inner product of equations valid for a given slice with expansion functions and use the orthogonality property of the expansion functions. As a result we arrive at [4]:

$$\begin{aligned} \underline{a}^n &= \underline{a}^{n-1} + \Delta t \underline{A} \underline{b}^{n-1/2} \\ \underline{b}^{n+1/2} &= \underline{b}^{n-1/2} + \Delta t \underline{B} \underline{a}^n \end{aligned} \quad (4)$$

where Δt is the time step, \underline{a} and \underline{b} are column vectors containing expansion coefficients for all slices and superscript n denotes the time step. The matrices \underline{A} and \underline{B} contain the inner products and have the following structure

$$\underline{A} = \text{qdiag} [\underline{A}'^k, \underline{A}''^k] \quad \underline{B} = \text{qdiag} [\underline{B}'^k, \underline{B}''^k] \quad (5)$$

The elements of the submatrices are given

$$\begin{aligned} A'_{ij}{}^k &= \langle (L_{1t}^k - L_{1z}^k) g_{j,k}, f_{i,k} \rangle & A''_{ij}{}^k &= \langle L_{1z}^k g_{j,k+1}, f_{i,k} \rangle \\ B'_{ij}{}^k &= \langle (L_{2t}^k + L_{2z}^k) f_{j,k}, g_{i,k} \rangle & B''_{ij}{}^k &= - \langle L_{2z}^k f_{j,k-1}, g_{i,k} \rangle \end{aligned} \quad (6)$$

Equations (4) show that expansion coefficients for all slices are updated at each time step as a result of mutual interactions of fields due to the inhomogeneity introduced by space dependence of constitutive parameters. As far as numerical cost is concerned, the most critical point in the PEE algorithm is the calculation of the inner products on inhomogeneous slices. However for inhomogeneous slices a classical FDTD algorithm can be used. Combining these two time domain techniques we create a hybrid method in which different algorithms are used in different parts of the computational space. The FDTD is used in the regions in which a fine resolution of field is necessary (eg. near edges, media interfaces) and the PEE is applied in the homogeneous subregions. This hybrid approach results in savings in numerical effort and computer memory. This is because the PEE is extremely efficient for homogeneous slices as matrices $\underline{A}'^k, \underline{A}''^k$ and $\underline{B}'^k, \underline{B}''^k$ are diagonal so that the computations are fast especially when the expansion functions are chosen in such a way that they constitute a set of eigenfunctions of the Laplace operator defined on 2D region forming a slice. In that case each expansion function satisfies the boundary condition and field equations globally over entire slice. As a result very few expansion terms are needed to accurately describe field at each slice. The FDTD and PEE algorithms are interfaced at a common slice. The transition from the FDTD to PEE is done in the following way. Given a field distribution at the $z = z_k$, provided by the FDTD part of the algorithm, the expansion coefficients at this slice are found by taking the inner product with each basis functions of the PEE. To switch from PEE to FDTD the series (3) are calculated at the interface plane at the points required by FDTD.

NUMERICAL EXAMPLE

In order to verify the hybrid algorithm the cutoff frequency of the EH_{11} of a rectangular guide loaded with a dielectric slab shown in fig.2 was computed and compared with the results obtained with a classical FDTD technique. For both algorithms the identical excitation, space discretization ($\Delta d = .5mm$), time step, and number of samples were assumed. The results are given in Table 1. For the FDTD algorithm alone the CPU time for the assumed discretization mesh was 53s. For the hybrid algorithm, the slab region was treated with the FDTD and the lateral homogeneous regions were calculated with PEE. The CPU time depends on the localization of the interface plane and the number of expansion functions used in the PEE part of the algorithm. When the interface is at $x_1 = 7.5$ and $x_2 = 12.5mm$, ie. when the FDTD mesh is terminated only one slice away from the inhomogeneous region, the CPU time of the hybrid algorithm varies from 18s (for 1 expansion function) to 27s (for 5 expansion functions), with most of the time (14s) consumed by the FDTD computations. The error introduced by low number of expansion function is the largest if only one term is used but for this structure is less then 0.1% compared the result obtained from pure FDTD calculations. interface plane. The error decreases as the interface plane is moved away from the inhomogeneity. This is due to the fact that higher order terms in the field expansion correspond to higher order waves traveling in the lateral direction. If the interface planes are located at $x_1 = 5$ and $x_2 = 15mm$, only one term in the PEE part is sufficient to obtain exactly the same results as with purely FDTD technique. The CPU time for this case is 31s of which 28s is spent in the FDTD part.

CONCLUSIONS

A new hybrid PEE-FDTD algorithm for the time domain analysis of electromagnetic waves in shielded structures was introduced. The obtained results indicate that it is possible to obtain the acceleration of time domain calculation by using the PEE algorithm in homogeneous parts of the structure. The results presented in this letter indicate that it is possible to obtain improvement in the speed of time domain computation of 3D and 2D shielded structures in which the homogeneous regions are predominant such as microstrip lines, coplanar guides, and discontinuities in planar guides.

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Table 1: Comparison of the results and CPU times (DELL 486/66) for the cutoff frequencies of EH_{11} mode in the 20 by 6 mm rectangular guide loaded with a dielectric slab $\epsilon_r = 2.5$, $w = 4\text{mm}$, $h = 4\text{mm}$ using a hybrid algorithm with number of expansion functions N and the localization of the interface planes as parameters

N	PEE-FDTD	Error rel. to FDTD	CPU FDTD part	CPU PEE part	CPU combined	Speed up rel. to FDTD (53s)
Interface of algorithms at $x = 7.5, x = 12.5$ mm						
1	20.2075 GHz	+ 0.1%	14s	4s	18s	2.9
3	20.1975 GHz	+0.05%	14s	9s	23s	2.3
5	20.1975 GHz	+0.05%	14s	13s	27s	1.96
Interface of algorithms at $x = 5, x = 15$ mm						
1	20.1875 GHz	0%	28s	3s	31s	1.7
3	20.1875 GHz	0%	28s	6s	34s	1.55

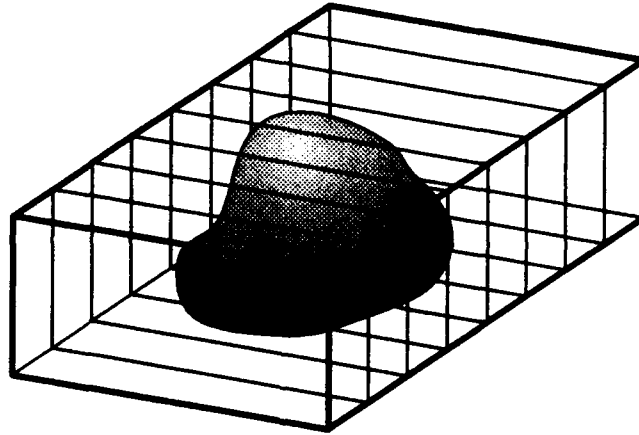


Figure 1: A structure discretized along one coordinate

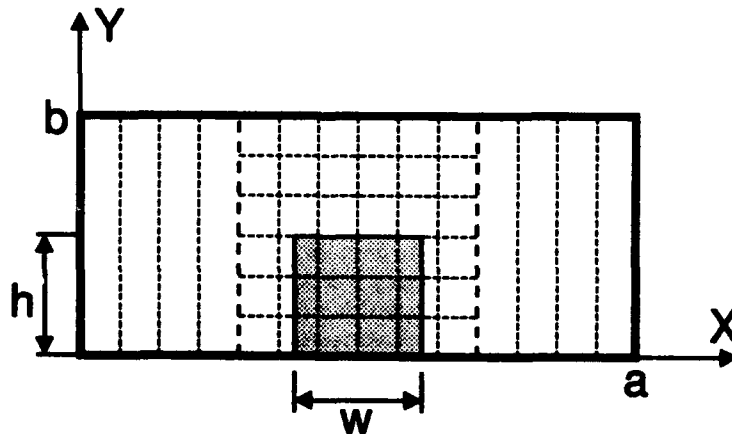


Figure 2: Geometry of the guide used in the numerical test showing FDTD and PEE meshes (Slab centered with respect to $x=a/2$, $\epsilon_r = 2.5$, dimensions: $h = 4\text{mm}$, $w = 4\text{mm}$, $a=20\text{mm}$, $b=6\text{mm}$)

**Stability Condition
for the Explicit Algorithms of
the Time Domain Analysis of Maxwell's equations**

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ABSTRACT

This contribution presents the derivation of the stability condition for various types of time domain algorithms used in the solution of linear hyperbolic differential equations which arise in the investigation of transient electromagnetic fields. The stability condition of the algorithm is derived by investigating the properties of operators in suitably defined Hilbert spaces. Compared to the classical von Neumann stability analysis, the functional analysis approach gives more general results which can be easily applied to some recent and possible future time domain schemes.

INTRODUCTION

Explicit algorithms for the solution of initial value problems have recently received much attention among researchers involved in the numerical analysis of electromagnetic fields. Two methods belonging to this class, known as finite difference-time domain (FDTD) and transmission line matrix (TLM) algorithms have intensively been developed in the last decade. Their salient feature is that electromagnetic field is analyzed in the time domain and the samples of relevant physical quantities at nodes located at the discrete points in space are used to represent a physical continuum. These two methods are constantly being improved. The improvements include the application of graded meshes or non orthogonal cells, application of local approximations or extension of the basic algorithms to the new class of materials such as ferrites or dispersive media. Also new concepts of space representation of fields have been introduced. Recognizing the progress achieved in the recent years in the time domain analysis of electromagnetic fields, it should be noted, that the explicit algorithms underlying these methods are not unconditionally stable and the improvements introduced to algorithms affect their stability. Consequently there is a need to investigate the stability criteria for new schemes [6]. In this contribution we shall present how stability of different algorithms can be investigated using functional analysis.

STABILITY ANALYSIS OF EXPLICIT TIME DOMAIN ALGORITHMS

Let us consider a hyperbolic differential equation

$$\frac{\partial^2}{\partial t^2} f + \mathbf{L}f = 0 \quad (1)$$

where \mathbf{L} is a linear differential operator. The hyperbolic equation of this type, supplemented by conditions at $t = 0$ can be solved for $t > 0$ using a classical finite difference explicit algorithm [2]. It is a known fact that the explicit algorithms are conditionally stable. The approach most frequently used to derive the stability condition is known as the von Neumann stability analysis [2, 5]. This analysis involves local expansion of unknown functions into Fourier series and assumes the finite difference representation of the operator. If \mathbf{L} is a Laplacian, the von Neumann approach leads the formula known as the Courant - Friedrich - Levy condition. More general results can however be derived using an alternative approach based on the functional analysis.

To investigate the stability of explicit algorithms for the hyperbolic equations it is useful to present a problem in a canonical form:

$$\Delta^2 t \mathbf{R} \frac{\partial^2}{\partial t^2} f + \mathbf{A} f = 0 \quad (2)$$

The time marching algorithm for the above problem is stable if the following conditions are fulfilled [1] (p.386):

$$\mathbf{A} = \mathbf{A}^* > 0, \quad \mathbf{R} = \mathbf{R}^* > 0 \quad (3)$$

$$\mathbf{R} - \frac{\mathbf{A}}{4} \geq 0 \quad (4)$$

In other words, for the time marching algorithm to be stable it is sufficient that both operators \mathbf{A} and \mathbf{R} are self adjoint and positive and additionally the operator $\mathbf{R} - 0.25\mathbf{A}$ is nonnegative. The canonical form (2) is obtained from (1) by simply writing it as

$$\frac{\Delta^2 t}{\Delta^2 t} \mathbf{I} \frac{\partial^2}{\partial t^2} f + \mathbf{L} f = 0 \quad (5)$$

Where \mathbf{I} is the identity operator.

Comparing (5) with (2) we get $\mathbf{R} = \mathbf{I}/\Delta^2 t$ and $\mathbf{A} = \mathbf{L}$. It can readily be verified that operator \mathbf{L} is symmetric and positive. It suffices to verify the condition (4). This condition is fulfilled when

$$\left\| \frac{\mathbf{I}}{\Delta^2 t} \right\| \geq \frac{\|\mathbf{L}\|}{4} \quad (6)$$

or

$$\Delta t \leq \frac{2}{\sqrt{\|\mathbf{L}\|}} \quad (7)$$

Thus the maximal time step in explicit time domain algorithms considered here depends on the norm of the operator \mathbf{L} .

For a self-adjoint bounded operator \mathbf{L} defined in the Hilbert space \mathcal{H} the norm is defined as [3]

$$\|\mathbf{L}\| = \sup_{y \in \mathcal{H}, \|y\|=1} |\langle \mathbf{L}y, y \rangle| = |\lambda_{max}| \quad (8)$$

where λ_{max} is the largest eigenvalue of \mathbf{L} .

STABILITY ANALYSIS FOR ONE DIMENSIONAL PROBLEM

One important conclusion which follows from the functional analysis approach is that the stability condition depends on how the unknown functions are represented. This is because the norm of the operator depends on the space it acts in. When solving a particular problem we choose the way the functions are represented and the criteria to measure the accuracy of our solution. This choice is equivalent to the choice of a functional space and affects the norm of the operator and thus the stability condition. To illustrate this problem in more detail let us consider a one dimensional problem

$$\frac{\partial^2}{\partial t^2} f - b(x) \frac{\partial^2}{\partial x^2} f = 0 \quad (9)$$

$$f(x, t_0) = f_0(x), \quad f(x=0) = f(x=l) = 0 \quad (10)$$

where $b(x) > 0$ is a time independent continuous function of x ,

One possible way of solving the above problem is to use a classical finite difference approach but let us find the solution by means of the method of moments. Let \mathcal{D} denote the domain

of operator \mathbf{L} and assume that it allows only square integrable functions satisfying Dirichlet conditions at both ends of the interval. By equipping the domain \mathcal{D} with an inner product

$$\langle u, v \rangle = \int_0^a uv \, dx \quad (11)$$

we specify it in terms of the Hilbert space. It can easily be verified that operator

$$\mathbf{L} = -b(x) \frac{\partial^2}{\partial x^2} \quad (12)$$

is positive and self adjoint. However if we would like to calculate its norm in this space we note that the operator \mathbf{L} is unbounded and consequently its norm is infinite. Its norm becomes finite however, if the operator is allowed to act in a finite dimensional space. This is what happens in practice because we always look for approximate solution to the problem using a finite number of elements to represent a function. Let us now expand the function $f(x)$ into series of basis functions

$$f(x) = \sum c_i f_i(x) \quad (13)$$

and use the inner product (11) to find the expansion coefficient at any instance of time.

The finite set of basis function defines the approximate finite dimensional subspace of original domain. Consider the following truncated set of basis functions

$$\sqrt{\frac{2}{l}} \sin \frac{i\pi x}{l} \quad i \leq N_M \quad (14)$$

The basis functions (14) span a finite dimensional space $\mathcal{H}_{N_M} \subset \mathcal{D}$ in which the approximate solution is sought for. Now it is easy to find the upper bound of the operator.

$$\|\mathbf{L}\| = \|b(x) \frac{\partial^2}{\partial x^2}(\cdot)\| \leq \|b_{max} \frac{\partial^2}{\partial x^2}(\cdot)\| = \|\mathbf{L}_m\| \quad (15)$$

Where b_{max} is the maximal absolute value of $b(x)$ over the interval $\langle 0, l \rangle$. The eigenvalues λ_i of operator \mathbf{L}_m are given by

$$\lambda_i = \frac{i^2 \pi^2}{b_{max} l^2} \quad (16)$$

and consequently the norm of \mathbf{L}

$$\|\mathbf{L}\| \leq \frac{N_M^2 \pi^2}{b_{max} l^2} \quad (17)$$

This leads to the condition

$$\Delta t \leq \frac{2l\sqrt{b_{max}}}{\pi N_M} \quad (18)$$

If we chose an alternative way and represent the function and the operator in a finite difference sense by specifying their values at discrete points the norm will be changed. If the discretization points are equidistant and the spacing is Δd then [1]

$$\|\mathbf{L}\| \leq \frac{4}{(\Delta d)^2 b_{max}} \quad (19)$$

yielding the Courant - Friedrich - Levy condition:

$$\Delta t \leq \frac{\sqrt{b_{max}}}{\Delta d} \quad (20)$$

APPLICATION TO ELECTROMAGNETICS

The stability analysis described above can be used in electromagnetic problems. Here the operator L can be specified as:

$$L = \frac{1}{\epsilon_0 \mu_0 \epsilon(x, y, z)} \nabla \times \frac{1}{\mu(x, y, z)} \nabla \times (\cdot) \quad (21)$$

(other definitions are also possible).

As an example let us consider a cube Ω with the dimensions $l \times l \times l$. In this region we seek an approximate solution to the hyperbolic equation with an operator defined by (21) given a finite number of expansion functions in the form of normalized products of sines and cosines

$$\sin \frac{i\pi\xi}{l} \quad \text{or} \quad \cos \frac{k\pi\xi}{l} \quad i, k \leq N_M \quad (22)$$

Let \mathcal{D} denote the domain of operator L . The basis functions (22) span a finite dimensional space $\mathcal{H}_{N_M} \subset \mathcal{D}$. We calculate the upper bound of the norm of operator $||L||$. Note that $||L|| \leq ||L_m||$. Where

$$L_m = (\epsilon_0 \mu_0 \epsilon_{min} \mu_{min})^{-1} \nabla \times \nabla \times (\cdot) \quad (23)$$

and

$$\epsilon_{min} = \inf \epsilon_r(x, y, z), \quad \mu_{min} = \inf \mu_r(x, y, z) \quad x, y, z \in \Omega \quad (24)$$

Using the same procedure as for one dimensional case we find the norm of operator L in \mathcal{H}_{N_M}

$$||L|| \leq ||L_m|| \leq v_{max}^2 \frac{3N_M^2 \pi^2}{l} \quad (25)$$

where $v_{max} = (\epsilon_0 \mu_0 \epsilon_{min} \mu_{min})^{-1/2}$ is the maximum velocity for a plane wave in the structure. Using the above estimation we get the following stability condition

$$\Delta t \leq \frac{2l}{v_{max} N_M \pi \sqrt{3}} \quad (26)$$

If the region Ω is a rectangular prism with the dimensions $a \times b \times l$ and the upper bound for i, l, m in the trigonometric expansion functions is K_M, L_M, N_M then the condition (26) becomes

$$\Delta t \leq \frac{2}{v_{max} \pi \sqrt{(\frac{K_M}{a})^2 + (\frac{L_M}{b})^2 + (\frac{N_M}{l})^2}} \quad (27)$$

Discretizing the space Ω in the z direction with the step Δd and using $K_M \times L_M$ sine and cosine basis functions to in the x and y directions, the stability condition derived using (19) is

$$\Delta t \leq \frac{2}{v_{max} \sqrt{(\frac{\pi K_M}{a})^2 + (\frac{\pi L_M}{b})^2 + (\frac{2}{\Delta d})^2}} \quad (28)$$

For the discretization of all three coordinates with steps $\Delta x, \Delta y, \Delta d$ we shall get the well known Courant condition [5]

$$\Delta t \leq \frac{1}{v_{max} \sqrt{(\frac{1}{\Delta x})^2 + (\frac{1}{\Delta y})^2 + (\frac{1}{\Delta d})^2}} \quad (29)$$

At this point it is interesting to observe that the derivation described above provides stability criteria for a few recently published time domain algorithms. For instance conditions (27) and (28) are the stability criteria for the Total Eigenfunction Expansion and Partial Eigenfunction Equations schemes derived in [8] (for sine and cosine basis functions). In a compact 2-D/FDTD algorithm described in [4] and investigated subsequently by Cangellaris [6], the functions are represented by samples at uniformly discretized cartesian coordinates x, y and the variation in

the z direction given in the form $\exp(-j\beta z)$. For this case the functional analysis approach gives

$$\Delta t \leq \frac{1}{v_{max} \sqrt{(\frac{1}{\Delta x})^2 + (\frac{1}{\Delta y})^2 + (\frac{\beta}{2})^2}} \quad (30)$$

This condition is identical as the one given in [4] and [6]. Also the stability of a hybrid spectral/FDTD method introduced recently by Cangellaris et al. [7] follows from condition (7).

CONCLUSIONS

The application of the functional analysis to the investigation of the stability of time domain algorithms has been presented. It was shown that the method can easily be applied to the investigation of the properties of novel time domain schemes for Maxwell's equations.

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